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# INFORMATION

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# BULLETIN



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89-09

## ACOUSTICS

**Boundary Element Conference--BEM 10** ..... David Feit 1

At this conference, the finite element method is challenged by the boundary element method as an engineering analysis and design tool.

**STRUCOME 88** ..... David Feit 4

STRUCOME (structures, conception, and measurements) 88 covered finite element analysis, boundary element analysis, and CAD/CAM.

## COMPUTER SCIENCE

**The Second International Conference on Quality Assurance and Standards in Finite Element Methods** ..... Michael A. Tuccio 7

The mission of NAFEMS is to promote the safe and reliable use of finite element technology. A forum is provided for discussing quality assurance issues.

**The 16th Annual International Symposium on Computer Architecture** ..... Ashok Singhal 11

Mr. Singhal summarizes the cache aspect of computer architecture, along with pipelined and parallel processors (including dataflow), mapping algorithms, networks, Prolog architectures, performance evaluation, logic simulation systems, and memory systems.

## CONDENSED-MATTER PHYSICS

**9th General Meeting of the Condensed-Matter Division of the European Physical Society** ..... Dean L. Mitchell 15

This increasingly important European forum for condensed matter physics featured such topics as surfaces and interfaces, semiconductors, superconductors, metals and alloys, disorders, and tunneling.

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The author discusses the conference goal--a new perspective on surface science.

## MATHEMATICS

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Dr. Franke describes work at the University of Rome in Mechanics and Aeronautics, and Mathematics Departments, and the parallel processing project at the University of Naples.

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Dr. Franke discusses six invited talks, and the panel discussion of compilers and languages.

<b>Surfaces in Computer-Aided Geometric Design</b> . . . . .	<b>Richard Franke</b>	<b>31</b>
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Meetings held at this research institute are prestigious, and invitations to participate are coveted. Dr. Franke provides valuable information about many presentations.

## PHYSICS

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This laboratory is one of four facilities in the world for user research capable of producing *dc* fields in excess of 30 tesla. Dr. Mitchell also summarizes other research efforts.

<b>Workshop on Compound Semiconductor Devices and Integrated Circuits in Europe</b> . . . . .	<b>Dean L. Mitchell</b>	<b>40</b>
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This article is presented in tandem with one by L.F. Eastman, Cornell University, giving two points of view--specialist by Eastman and semi-conductor physics by Mitchell.

<b>Workshop on Compound Semiconductor Devices and Integrated Circuits in Europe</b> . . . . .	<b>L.F. Eastman</b>	<b>42</b>
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This article, presented in tandem with Dr. Mitchell's article, gives highlights of the workshop.

<b>Detonics Research and Development in France--A Discussion with General Jean Boisson, Armament Inspector for Powders and Explosives of the French Ministry of Defense</b> . . . . .	<b>Marco S. Di Capua</b>	<b>43</b>
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Dr. Di Capua divides detonics research in France into three areas--the French Atomic Energy Commission, the Ministry of Defense, and private industry--and briefly discusses each.

<b>The Plasma Physics Laboratory at École Polytechnique, Palaiseau (Paris), France</b> . . . . .	<b>Marco S. Di Capua</b>	<b>45</b>
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École Polytechnique research concentrates on areas that fit closely with research efforts at French national laboratories, universities, industry, and military research organizations. The research is also coupled with efforts abroad, especially in Z-Pinches laser-matter interactions, and free electron lasers.

<b>NATO Advanced Study Institute on Scanning Tunneling Microscopy-- Physical Concepts, Related Techniques, and Major Applications</b> . . . . .	<b>Marco S. Di Capua</b>	<b>48</b>
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The purpose of this meeting was to provide a forum to help understand the basics of STM, to identify and discuss common applications, and to discuss new approaches.

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<b>Influence of the Minority on the Majority</b> . . . . .	<b>William D. Crano</b>	<b>66</b>
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This conference focused on research on the factors that foster the impact of a minority group on the actions and beliefs of a majority group.

## SOLID-STATE PHYSICS

<b>Condensed-Matter Research at the École Polytechnique</b> . . . . .	<b>Dean L. Mitchell</b>	<b>71</b>
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Dr. Mitchell reports on photoemission and fractals research at the Laboratoire de Physique de la Matière Condensée of the École Polytechnique.

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# ACOUSTICS

## Boundary Element Conference--BEM 10

by David Feit, the Liaison Scientist for Acoustics and Mechanics in Europe and the Middle East for the Office of Naval Research European Office. Dr. Feit is on leave from the David Taylor Research Center, Bethesda, Maryland, where he is a research scientist in the Ship Acoustics Department.

The finite element method (FEM) is now used in almost every sphere of scientific calculations, and is considered by some to be the most important numerical technique used in engineering analysis today (Strang, 1986). However, I believe that several participants at BEM 10, the tenth in a series, held at Southampton, U.K., would challenge this notion, and proclaim that the Boundary Element Method (BEM) can offer a serious challenge to FEM as an engineering analysis and design tool (Bebbia, 1988).

This conference, like all the others in the series, was organized by the Computational Mechanics Institute, Ltd. (CMI), Southampton, U.K., Dr. Carlos A. Brebbia, Director. For more than 10 years, Brebbia has been a principal developer and proponent of BEM.

The CMI, located at Ashurst Lodge in the New Forest just outside Southampton, provides information, computer codes, and training to the engineering industry. It is organized into three divisions--a division that develops and markets computer software based mostly on the BEM; another division that publishes journals, proceedings of conferences, and books devoted to computational aspects of mechanics; and the Wessex Institute of Technology that serves as an educational institute. According to Brebbia, the latter has been chartered to grant advanced degrees recognized by the Center for National Academic Awards (CNAA). On a visit to CMI, separate from my attendance at BEM 10, I was introduced to several graduate students working on doctoral theses using BEM in a variety of problems related to mechanics. My impression was that they were principally from the Far East and South America where Brebbia seems to have many contacts and much influence.

During the 3-day BEM 10 conference, there were some 135 papers presented and nearly 200 attendees from locations including Australia, Asia, and South America, as well as Europe and North America. The papers covered all aspects of the BEM, ranging from fundamentals to applications. Some of the session titles were

- Mathematics and computational aspects
- Heat transfer
- Fluid flow
- Electrical applications
- Geomechanics
- Wave propagation
- Vibrations
- Stress analysis.

In addition, there were several special tutorials on such subjects as the application of BEM to nonlinear diffusion, nonlinear material problems, to wave propagation, and to acoustics and noise control.

### Opening Remarks

Carlos Brebbia presented the opening remarks in which he talked about the recent 10-year period during which the BEM has been developed into a practical engineering tool. Brebbia stated that the BEM can now challenge the pre-eminence of FEM in analysis and design of mechanical systems. He also said, "...boundary elements is a new and more powerful technique than finite elements, and that the latter can be seen as a particular case of BEM rather than the other way round." I imagine that this might be disputed by those who have been developing and advocating the use of FEM over the last few decades. As an outsider to the field, I imagine that each of the methods has its advantages and disadvantages. A principal advantage of the BEM over FEM is that the former only requires that the bounding surface of a problem be discretized as opposed to the volume in the latter. Of course, there are concomitant disadvantages such as the nonlocality of the equations arising out of the procedure caused by the long range influence of the Greens functions used in the formulation. This results in matrices of influence coefficients that are fully populated. There are some problems such as the structural acoustics problem of a vibrating structure in an unbounded acoustical medium, which could undoubtedly be best served by an approach utilizing a combination of the two methods.

Brebbia concluded his remarks by enjoining BEM practitioners to be more audacious and innovative in their approaches to fully realize the potential of the method, especially in the areas of nonlinear and time-dependent problems.

## Mathematical and Computational Aspects

Some of the papers in this session principally addressed the applicability of BEM methods to nonstandard problems such as nonlinear cases and elastoplasticity.

The paper by N. Tosaka and K. Kakuda, Nihon University, Narashino, Japan, discussed the application of the generalized BEM for nonlinear problems. Their approach uses the fundamental solution or Greens function for a linearized version of the nonlinear equation being solved which is then applied to each subdomain of the problem. This fundamental solution contains the unknown function implicitly. The final set of matrix equations is constructed by combining the equations of each subdomain and enforcing compatibility of the solution and its derivatives at the subdomain boundaries. This leads to a set of banded matrix equations of a quasi-nonlinear variety. An iterative solution to solve this problem is proposed and applied as an example to two one-dimensional nonlinear differential equations of the second order.

C. Polizzotto, University of Palermo, Italy, showed how the classical mixed-type variational principles; e.g., those of Hu-Washizu or Hellinger-Reissner, can be used in the application of BE to elastoplasticity theory. Symmetry and positive definiteness of the coefficient matrix of the resulting equations are the main features of these formulations. Colonnetti's principle allows the same BE formulation as that of the elastic system under the action of external forces and the unknown plastic strains treated as initial strains, with the body discretized into cell elements (CE) to model the material plastic behavior. The plastic yielding laws for single CEs are derived using the Hill maximum work dissipation theorem. The mathematical programming procedures of engineering plasticity can then be used to solve the resulting discretized structural system set of equations.

Several other papers discussed finding the appropriate variational principle that would lead to matrix equations on the unknowns having symmetric coefficients. Such sets are generally more computationally efficient and lead to simpler numerical procedures when coupling to finite elements are necessary. In particular, the paper by E. Schnack, I. Becker, and N. Karaosmanoglu, Karlsruhe University, Karlsruhe, Federal Republic of Germany (FRG), showed the advantages of coupling the two methods, BEM and FEM, in certain problems where, for

example, one part of the domain is subject to high gradient fields, such as those caused by cracks. Here it is suggested that it is better to use BEM in the domains including the cracks where the high gradient fields are expected. A comparison example was done using each of three methods--BEM, FEM, and coupled BEM/FEM. In this example, which was a three dimensional (3-D) elasticity analysis of a plate with a hole under tension, the coupled BEM/FEM approach gave excellent results with the lowest CPU time.

In another invited paper, E.P. Stephan, Georgia Institute of Technology, presented error estimates for the h-p version of the Galerkin BEM for the solution of integral equations on polygons and open arcs using a variety of meshing schemes. In the h version, accuracy is achieved by decreasing the mesh size h, keeping the order p of the piecewise polynomials fixed. In the p version, a fixed mesh size is used with increasing p, while the h-p method combines the two approaches.

From my perspective, the most interesting part of the conference dealt with the applications of BEM to geomechanics, wave propagation, and vibrations. Most of these papers appear in Volume 4 of the Proceedings. I shall now discuss some of the papers presented in these sessions.

## Geomechanics

D.E. Beskos, University of Patras, Greece, gave the opening invited talk. Beskos reviewed boundary element formulations for the numerical solution of geomechanics problems. Advantages of this approach are: dimensionality reduction, high accuracy, easy treatment of infinite or semi-infinite domains, the successful stress analysis of cracked bodies, and the efficient solution of 3-D problems. Beskos surveyed and cited papers in geomechanics using BEM covering the specific areas of foundations and piles, mining and excavation, soil consolidation, wave propagation, and dynamic soil-structure interaction. Citations and references total 191.

H. Antes, Technische Universität Braunschweig, FRG, and B. Steinfeld, Ruhr-Universität Bochum, FRG, discussed unilateral contact problems in dynamic soil interaction by a time domain BEM. Unilateral contact problems are special in that some of the boundary conditions are presented over a domain which itself must be determined in the solution of the problem. When the external forces are transient, then the time step of contact or separation also must be determined. The time domain BEM is applied to two problems--one is a heavy dam-soil system under a vertical impulse, while the other considers the same system excited by a horizontal impulse.

D.E. Beskos was either the author or coauthor of three papers within this session, and in the last paper coau-

thored with G.D. Manolis, State University of New York (SUNY), Buffalo, he discussed the boundary integral equation formulation for dynamic poroelasticity. Biot's equations of dynamic poroelasticity in the Laplace transformed domain are used to formulate the appropriate boundary integral equations. To do this, it is first necessary to obtain the fundamental solutions of dynamic poroelasticity and these are constructed. These are shown to reduce to the fundamental solutions of elastodynamics. No specific problem applications were discussed in this presentation.

## Wave Propagation

R.P. Shaw, SUNY, Buffalo, gave an overview of the various boundary integral equation formulations that can be used in the case of time-harmonic scattering of acoustical waves. During the opening session of the conference, R.P. Shaw received an honorary medal from C. Brebbia for his pioneering work in BEM. (On a personal note, my doctoral thesis work at Columbia University followed up on the Shaw's thesis, who preceded me by a few years at Columbia. Although I did not realize it at the time [the BEM approach had not been formalized yet], I also had applied the BEM to an elastic solid-fluid wave interaction problem very early in my career.)

The BEM in these applications is very advantageous since it eliminates consideration of the infinite fluid domain and concentrates its action on a finite bounding surface of the problem. Shaw first reviewed the various integral equation formulations used in time-harmonic acoustic scattering or radiation problems, and then discussed the methods used to solve the resulting integral equations. In addition to "element" solutions, he discussed the T-matrix method which assumes the solution in terms of a series expansion valid over the entire extent of the boundary. One difficulty that arises in these type problems is that the boundary integral equation approach to these exterior acoustical problems seems to fail at specific frequencies corresponding to the eigenvalues of the interior problem for the same geometry. Shaw also discussed several approaches that have been introduced to circumvent this difficulty. He then discussed the relative merits of the BEM method versus the T-matrix method, but concluded that the two approaches are to be viewed as complementary and the choice of one over the other is more a question of personal preference rather than the inherent superiority of either.

## Acoustics

P.J.T. Fillippi, Laboratoire de Mecanique et d'Acoustique, Marseille, France, reviewed the use of BEM in acoustics and vibrations over the last twenty years. The

examples discussed included: the eigenfrequencies and pressure fields in a bounded domain, diffraction of a sound wave by a thin screen, wave propagation over a ground plane with impedance discontinuities, eigenfrequencies of thin elastic plates, and sound radiation by baffled plates and cylindrical shells. Fillippi also described the principle advantage of the method for acoustical problems in terms of the reduction in dimensionality of the problem to a finite boundary domain, and the use of an explicit fundamental solution as the influence function in the boundary integral equations; i.e., the numerical approximation is made on the boundary conditions itself rather than the functions appearing in them.

In this session, several other papers gave more specific examples of using BEM in acoustics and noise control problems.

The paper by S. Amini and K. Chen, Plymouth Polytechnic, Plymouth, U.K., discussed the use of iterative techniques for the numerical solution of the second kind of Fredholm integral equations that arise in acoustical problems. In particular, they discuss the applicability of the conjugate gradient method, two-grid methods, and more general multi-grid methods. The iterative methods discussed were applied to two test problems, one being the exterior Dirichlet problem for the two-dimensional Helmholtz equation (wave equation), where the boundary surface is an ellipse. The different computing methods for the solution of the resulting boundary integral equation were employed with the multi-grid methods turning out to be the most efficient for the problem discussed.

A. Seybert, University of Kentucky, showed how BEM is applied to practical noise control problems. The applications included automobile muffler design problems, and the prediction of noise radiated by vibrating structures such as engines and transmissions. Seybert has now packaged his software into a commercially available code specifically using BEM for acoustical problems. There are also a few European companies now marketing software directed to acoustical noise control and radiation problems.

## Conclusion

This meeting introduced me to the BEM field and to a new group of applied mathematicians and scientists working in this field. I was impressed by the wide-ranging number of countries from which the participants came to present papers indicating the very wide-spread introduction of BEM technology.

Although I was aware of the use of boundary integral equation methods, I was less aware of the extent of problems that have been formulated and solved using the BEM specifically. For structural acoustical problems in-

volving vibrating structures radiating or scattering sound waves, the BEM is very advantageous. Since such meetings are held on a yearly basis, I would highly recommend that others interested in computational solutions to structural acoustical problems follow up on this series.

The Proceedings are available as a set of four volumes and can be ordered from Computational Mechanics Publications, Southampton, U.K.

## References

G. Strang, *Introduction to Applied Mathematics*, Wellesley-Cambridge Press, 1986.

C.A. Brebbia, Editor, *Proceedings of Boundary Elements, Vol. 1, Mathematical and Computational Aspects*, Computational Mechanics Publications, Springer-Verlag, 1988.

# STRUCOME 88

by David Feit

## Introduction

As the design process in engineering looks more and more to the optimizing of engineering structures, computer aided techniques such as Finite Element Analysis (FEM), Boundary Element Analysis, and Computer Aided Design and Manufacturing (CAD/CAM), become paramount. A survey in March 1988 of readers of the French technology magazine "Industries et Techniques" found that 71 percent of the respondents regularly use computers for their structural calculations, while only 22 percent still rely on their personal calculations.

Within such an environment, AS&I DATAID and the publishers of "Industries and Techniques" organized the STRUCOME 88 meeting held at the Paris Palais de Congres, November 2-4, 1988. STRUCOME is an acronym for the phrase *Structures, Conception, and Measurements*. The conference not only covered FEM and CAD/CAM, but also added the new theme *measurements*, to include discussion of the use of experimentally obtained measurements to aid the design process.

More than 80 European papers were selected for the 3-day conference and were presented to some 350 participants. The primary aim of the conference was to present the state-of-the-art in FEM, CAD/CAM, and most importantly, from my perspective, the use of vibration measurement integrated with FEM. Each of the three topics was introduced by internationally known experts in the respective fields--O.C. Zinkiewicz, P. Bezier, and D.J. Ewins.

In his welcoming remarks STRUCOME General Secretary, H. Debaecker, stated that the meeting "...is now determinedly orientated towards Europe" and supported by the European Community. Although the meeting was held in France and organized by French institutions, the official languages of the meeting were French and English with simultaneous translations of talks advertised to

be available. Unfortunately, translations were available for only the major introductory talks and those talks presented in one of the three or four lecture rooms used for parallel sessions.

The topics covered included the applications of FEM to

- Large displacements
- Optimization of structural design
- Acoustics, piezoelectricity, and magnetism
- Dynamics and vibrations
- Composites
- Meshing
- Dynamic measurements, and correlations between tests and theory
- Recent software developments.

I shall review the introductory lectures and a selected number of papers most relevant to acoustics, and structural dynamics calculations.

## Introductory Lectures

O.C. Zinkiewicz, University of Wales, Swansea, U.K., a pioneer in finite element analysis, began with a short history of computational mechanics stressing that it developed to help engineers solve practical problems. According to Zinkiewicz, physicists investigate the physical world as it is, whereas engineers must deal with what has never been. He attributed the first example of using computational mechanics to Richardson in 1908, and then jumped to Southwell's development of *relaxation* techniques to solve linear sets of equations in 1943. In terms of current developments, Zinkiewicz talked about the importance of data presentation and the wide spread use of data visualization techniques such as color coding of the solutions. I think that I noted a hint of criticism when he talked about how "...color impresses," but that

sometimes results are presented with "...no regard for accuracy." In his view, some FEM users are too little concerned with accuracy. Zinkiewicz also discussed error estimation and automatic mesh generation to reduce errors, and the three R's necessary for computational methods--Range, Robustness, and Reliability.

P. Bezier, engineer of the "Ecole des Arts et Metiers" and well known for his work in the field of computer-aided design, presented the second plenary lecture. In particular, he is noted for his work in the modeling of complex surfaces, and these are now known as Bezier splines and surfaces. His talk was historical talking about the early difficulties in specifying the topographical aspects of practical surfaces used in the automobile industry. These efforts began in the early 1960s with the requirement of mathematically specifying three-dimensional shapes arising from designers' drawings or physical models. The talk had more of the flavor of reminiscences of his career and less technical content than the other plenary lectures.

D.J. Ewins, Imperial College, London, presented the last plenary lecture and discussed the subject of modal testing. Ewins is a well-known expert in this field, having written a book, *Modal Testing: Theory and Practice*, and organized several *roundrobin* test programs related to the dynamic response of structures. While acknowledging that modal testing is widely used, Ewins stressed the fact that it is not always done well or developed as well as it could be given our present knowledge of FEM. Modal testing can be used to describe the dynamic behavior of a structure by determining its mathematical model (mass and stiffness distribution) from experimental results. Unfortunately, the model so derived is much less complete than that which could be determined analytically. Because it is expensive to do modal testing of large and complex structures, it is necessary to extract maximum benefit from the time spent.

After discussing such generalities, Ewins discussed the results of *roundrobin* testing of a structure consisting of a cylinder on isolation mounts. For this particular exercise, computations were also done in parallel and compared to measured results. As expected, the number of calculated resonances exceeded the number measured. Twenty laboratories participated, but only 15 responded. The conclusions were that poor comparative results can be derived if the techniques of modal testing are not used properly, and the optimum strategy is to use both analytical and experimental methods side by side.

### Applications of FEM to Acoustics, Piezoelectricity, and Magnetism

The first paper in this session was written by J.P. Coyette, P. Guisset, and E. Dejehet representing Dynamics Engineering, a Belgian company with offices in

France and the U.K. This company, like a number of other European companies, has developed a computer program for the numerical modeling of exterior acoustical problems (also can be used for the interior acoustical problem which is somewhat easier to implement). This program models the exterior acoustical problem using the surface Helmholtz integral representation in which the surface pressure is written as a function of the surface velocity. The usual treatment of such an equation is based on a collocation scheme that has two principal difficulties. One is caused by singularities in the integrals and the other is that the resulting system of matrix equations has unsymmetric coefficients. The approach used here makes use of a formulation introduced by Hamdi (Hamdi, 1982) which leads to a matrix equation with symmetric coefficients, but one still has to get around the problem of dealing with singularities in the integrals.

Several applications are discussed--the pulsating sphere problem which exemplifies a *critical frequency* problem, and rigid piston mounted on a rigid box. The advances described in this paper include using refined iso-parametric surface elements, selective and adaptive integration rules, symmetrization of the matrix, and a concise treatment of the *critical frequency* problem. All of these features are incorporated into a software package available from Dynamics Engineering; the package is marketed under the name SYSNOISE. I understand that this package has been sold to and used by a ship design firm working under contract to the French Navy.

METRAVIB RDS, a French acoustical research and development firm headquartered in Lyon, was well represented at this meeting and especially in this session where there were two papers on structural acoustics presented by its staff members. The first by D. Doizelet, J. Larcher, and J. Parot treated the diffraction of acoustical waves by an elastic screen. The approach here, like that of the preceding paper, also uses the Helmholtz integral representation to relate the pressure and particle velocity on a bounding surface of the problem, thus eliminating the need to model or determine the acoustical field over the entire volume of the domain. The pressure differential in the above equation is related to the dynamic response of the structure representing the screen, and this can be approximated using a finite element representation of the screen velocity. The problem is then reduced to that of solving a coupled set of two integrodifferential equations relating the surface acoustical pressure and the normal velocity. Without discussing the details of the program, the authors presented specific results for the problem specified earlier in this paragraph, and show good agreement with what they say is an analytical formulation (Houcine, 1985).

C. Avallet, METRAVIB RDS, discussed the program GAP that has been developed to calculate the vibrational response and acoustical radiation from shells equipped

with internal structural systems. The shells are cylindrical and can be stiffened by internal frames. The problem is broken up into two subproblems--the stiffened shell immersed in water, and the system of internal equipment. The approach consists of calculating the receptances of each system at the attachment points and then calculating the global response using the equations of compatibility. The shell is modeled using a transfer matrix approach developed from classical thin shell equations (Leissa, 1973), and the external fluid is modeled using finite differences in the radial direction and assumed to be periodic in the axial and circumferential directions. No specific results were presented other than a general discussion of the convergence properties of the point receptances compared to the transfer receptances for low and high frequencies (as compared to the cylinder *ring frequency*). The Service Technique des Constructions et Armes Navales (STCAN) and the Centre d'Etudes et de Recherche sur la Discretion Acoustique des Navires (CERDAN) sponsored the work.

The U.K. was represented in this session by a paper written by R.D. Henshell and P.C. Macey, PAFEC Ltd., Nottingham, and presented by R.D. Henshell. This company has developed a large scale structural analysis system marketed under the name PATRAN. The paper discusses a structural acoustic capability that has been recently added to their system. The paper reviewed very briefly all the principal numerical techniques that have been used in the general structural acoustic problem. The techniques include: modeling of the acoustical fluid using fluid finite elements; the virtual mass approximation wherein the fluid/vibrating structure interaction is modeled assuming that the fluid is incompressible (usually most appropriate in the low frequency range); the plane wave approximation (the surface pressure is proportional to the surface normal velocity); the Doubly Asymptotic Approximation (Geers, 1983) which in effect combines the two previous approximations; and the exact boundary element formulation (previously described in the discussion of the first two papers in this subject). Although not mentioned specifically in this paper, I believe that the acoustical package developed by PAFEC can implement any of the above formulations which are at the option of the user. In a recent exercise, I have asked for and received calculations from PAFEC on the specific problem of scattering of acoustical waves from a cylindrical shell; in this application, the boundary element formulation was used. The results compare favorably to those obtained from independent calculations.

### Correlation of Modal Testing and FEM Model Results

It is sometimes very useful to make refinements to an FEM model of a structure based on experimentally derived data obtained from a prototype structure. Such

modifications have been going on for many years in a wide range of applications, including those of aerospace vehicles, but the consensus of the community seems to indicate the results are of uncertain quality. In an effort to examine the problem in a more systematic way, a European-wide action group has been formed--Action Group 11 (AG 11) of the Group for Aeronautical Research and Technology in Europe (GARTEUR). The GARTEUR is comprised of individuals from the Federal Republic of Germany, France, the Netherlands, and the U.K. These individuals are drawn from either academia, government research laboratories, or industries, and funds come from the institutions represented by the individuals. Dr. R. Ohayon of the French Office Nationale de Etudes et Recherches Aerospatiale (ONERA) is chairman and Dr. D. Ewins (referred to earlier in this report) is vice chairman. Some of the group made presentations at this meeting. I shall discuss one of the papers presented by one of the members of the group. I am keeping abreast of the activities of this group and will be reporting on them in future ESNIB issues.

M. Nash, Royal Aerospace Establishment (RAE), Farnborough, U.K., discussed the general problem of adjusting a finite element model to reproduce the results of model testing. Nash then described the procedures that are used at RAE and applied them to the exercise that has been organized by GARTEUR (see ESNIB 89-07:58).

The model problem consists of determining the planar vibration modes of a reference simple truss model with specified mass and stiffness properties. The *measured* data consists of specified frequency response data at a reduced number of measurement points; i.e., 78 degrees of freedom (dof) problem compared to 234 dof of the reference finite element model. The numerical results for the reduced problem were determined in the presence of known modifications to the stiffness distribution. Each participant was asked to use whatever procedures they had experience with to determine what the modifications were so that they could update their FEM model after localizing the model errors. The error localization techniques used by RAE were calculation of mode difference vector, flexibility error matrix, stiffness and mass error matrices, stiffness difference matrix, and dynamic force residue. The results from these procedures were reviewed and collated to determine the most likely source of error and the FEM model was adjusted in light of these errors. Finally, the adjusted model was compared to the exact modified model used by ONERA to generate the original *measured* data results.

### Conclusion

From this meeting, I came away with the impression that there is a widespread use of computers in the design

and analysis of structures within France. Many companies are supplying software for this purpose, and it was evident at this meeting that there is a large market for such programs. On another note, I also became more aware that the French are making a concerted effort at joining in with other members of the Economic Community to promote the use of computer techniques in engineering, and that there are cooperative efforts underway to make sure that such techniques are not used unwisely nor abused.

## References

Geers, T.L., and C.A. Felippa, "Doubly Asymptotic Approximations for Vibration Analysis of Submerged Structures," *J. Acoust. Soc. Am.* 73, No. 4, 1983, 1152-1159.

Hamdi, M.A., "Formulation variationnelle par équations intégrales pour le calcul de champs acoustiques linéaires proches et lointains," These d'état, Université de Technologie de Compiègne, 1982.

El Houcine, J., "Applications des méthodes d'équations intégrales à l'étude numérique de la diffraction du son par un obstacle," These de Doctorat, University Claude Bernard, Lyon I, 1985.

Leissa, A.W., "Vibration of Shells," NASA SP-288, 1973.

# COMPUTER SCIENCE

## The Second International Conference on Quality Assurance and Standards in Finite Element Methods

by Dr. Michael A. Tuccio, Applied Mechanics Division, Engineering Department, Naval Underwater Systems Center, New London, Connecticut.

### Background

The National Agency for Finite Element Methods and Standards (NAFEMS) is a work program began in 1983 by the National Engineering Laboratory (NEL), Glasgow, U.K., and supported financially by the Department of Trade and Industry. The mission of NAFEMS is to promote the safe and reliable use of finite element (FE) technology. The NAFEMS is expanding and intends to develop its business potential as part of Prime Minister Thatcher's privatization plan. Its publication, *Benchmark*, is growing into the leading specialist magazine for the FE user. In the early years of NAFEMS, industry was wary that the organization would be a government controlling agency. However, experience has shown that NAFEMS provides an excellent forum for the discussion of quality assurance (QA) issues and has been embraced by industries throughout Europe. Similar organizations exist in the European Community (EC) such as the French National Committee Validation des Programmes de Calcul de Structures (Validation of Structural Analysis Software) of the Société Française des Mécaniciens (SFM) created in 1987. In the U.S., a similar effort was begun by the engineering professional societies--ASME, AIAA, ASCE--but never gained acceptance because of similar concerns of government control. However, many

major U.S. players have maintained working relationships with NAFEMS.

### Introduction

The second International Conference on Quality Assurance and Standards in Finite Element Methods took place at Stratford-upon-Avon, U.K., May 22-25, 1989, hosted by NAFEMS. Most of the attendees were from the EC, with Yugoslavia, Canada, and the United States were also represented. (No list of attendees was available so there may have been representatives from additional countries.)

Proceedings were published in advance and were available to attendees at registration. The conference organization was excellent because of the efforts of George Leckie and Ann Crecham, NAFEMS.

The Finite Element Method (FEM) is being taught in European undergraduate schools. In discussions with several of the delegates from universities, FEM is introduced to 2nd, 3rd, or 4th year students depending upon the institution. This contrasts with the U.S. in that the FEM is not taught at the undergraduate level at most universities (from my perspective).

### Discussion of Papers

All of the papers discussed the accuracy and error analysis from various points of view, but were mainly con-

cerned with both the finite element behavior, and mesh generation problems. There was also unanimity expressed that the accuracy of FE analysis can be controlled and predicted with confidence.

Professor O.C. Zienkiewicz, Swansea, U.K., gave the keynote address in which he discussed error estimates and adaptivity. Zienkiewicz is one of the world's leaders in the development of the FE method and is a member of the Royal Academy of Science. The thrust was that the analyst must understand the acceptable error a-priori in order to take the full benefits of the analysis. Then, if the desired accuracy of the original computations is not available, the analyst must be informed on how such accuracy can be reached and what kind of discretization approximation will do it most effectively. (Error is based upon the deviation from average stress values within the element.) It is possible to do this in the context of artificial hierarchical p-refinement; e.g., element order mesh refinement. And possibly, in conjunction with the currently acceptable h-refinement; e.g., element size mesh refinement, must be taken into account at the cost of scrapping much of the existing software.

"Quality Assurance of Mechanical Applications and Software: A Contribution to Nuclear Safety" by J.R. Levesque, the Electricite de France, presented the viewpoint that the principal objective for software QA is to give confidence in using a particular code and delimiting its validity domain. The software QA must follow this plan: specification-conception-coding-documentation-integration and tests global validation. In other words, QA must be part of the objective at the outset of any software development. As an aside, Levesque noted that the French are also trying to include experimental test results as well as numerical analysis results in QA. This brought considerable debate, especially from the U.S., in that there seemed to be a predominance of "QA by numerical analysis only" opinions in the comment session.

The first presentation from an industrial author entitled "The FE Quality Assurance Program in Lucas Industries" was given by Lees. The theme was that although a trend toward general increased awareness of QA has been visible over recent years, it is still imperative that the messages are widely distributed both to users and managers. Unless local management fully appreciates the importance of FE QA, they will not support the time and cost of the necessary training courses. Now that low-cost personal computer-based FEA packages are available, it is particularly important that the FE QA issues be addressed throughout the organization.

Trajanovic, University of Nis, Yugoslavia, described the classification of the potential error sources in the structural analysis process by the FE method. The structural analysis process itself is chosen as the classification basis. Based upon the classification, the sources of errors were analyzed regarding their cause. The analysis

showed that the errors in results could be significantly reduced by using an intelligent preprocessor that would be based upon the qualitative knowledge base; e.g., artificial intelligence.

The first invited lecturer was R.B. MacNeal, MacNeal-Schwandler Corporation, who spoke on "A Single Element Test for Membrane Locking." Membrane locking is a condition of excessive stiffness that occurs only in curved shell elements. The condition is characterized by the presence of unwanted membrane strains in loading conditions that should produce only bending. The root cause of membrane locking is that shape functions of at least cubic degree are required to describe the displacements caused by bending of a curved element. Thus, elements with one edge node per side are particularly susceptible to membrane locking. MacNeal proposed a single element test based upon the analysis of a quarter of a hemisphere with a hole at its apex subjected to concentrated loads at its equator. The new test has revealed that whereas the 3- and 6-noded triangular elements and the 4-noded Quad4 elements performed well, the Quad8 element has membrane locking modes associated with bending in the cross-curvature direction. It is likely that other 8- and 9-noded elements which employ reduced order integration of membrane strains exhibit similar membrane locking modes.

A seemingly controversial paper, presented by John Aas, FEGS Ltd., U.S. entitled "Computer Integrated Manufacturing (CIM) Has Come to Stay. Is FEM Part of the Solution or Adding to the Problems?", did not stimulate as much discussion as I had anticipated. According to the author, analyses based on computer simulation using FEM are comparatively slow. The functionality of FEM cannot support the speed and dynamics of model changes found when using computer-aided design (CAD). To include FEM technology in the CIM strategy, the FEM and its use must adapt to the new requirements set by CAD-based product design. The major obstacle today is a technical gap between data structures used in the different systems. Research into compound boundary representations and automatic hexahedral meshing is necessary to establish a credible solution. An FEM solid modeler, where discretization phase is hidden to the user will be a halfway stage, was proposed by the author and I expected to hear gasps in the audience, but I saw a lot of nods.

Armstrong, Rolls-Royce Plc, U.K., presented a paper on FEM automation entitled "Fully Automatic Analysis in an Industrial Environment." Automatic analysis is complete automation--from preparation of the numerical approximation to the physical mode, solving the equations, estimating the validity of the numerical approximation, and finally modifying, if necessary, to get a converged solution. The system he described is targeted at a 15-minute interval from receipt of geometry to inter-

rogation of converged results. An interesting comment by Bathe: "Automatic procedures would alleviate the analyst from the burden of establishing appropriate meshes for accurate analysis results so that he/she can concentrate fully on the actual design process and employ finite element procedures truly as only a means to find better design solution."

Afzali, CETIM, France, concentrated his remarks on the QA procedures applied to software production in his paper, "Q/A of Software Procedures Used in Castor Development." Afzali broke the procedure into three areas--documentation, software validation, and maintenance. In documentation, one must use substantial on-line documentation with descriptions of routines as well as the following formal manuals: programmer, software specification, global and detail design, theoretical, users, and test. The software validation test should contain routine functionality tests, sample accuracy tests, semi-industrial tests. In addition, the reference tests among those by NAFEMS or SFM/VPCS should also be performed. Afzali maintained that the software should help the users by offering tools such as error estimation and eventually autoadaptive mesh refinement.

On the second day, the invited lecturer was R. Brown, retired head scientist, Hughes Aircraft, U.S. Brown pointed out the need for canonical data structures and object-oriented data bases that would be accessed by object-oriented languages to reduce the number of lines of code. These would be similar to programs such as "Mathematica", which allow symbolic manipulation of instructions. This futuristic look at how the FEA world could benefit by such thrust was very exciting especially when one realizes that many necessary tools are already available.

Standards were discussed by several authors, but Mead et al., presented "The CAD\*I Standard for Finite Element Data Exchange," which explained this particular neutral format. As background, in 1984, the European Strategic Program for Research and Development in Information Technology awarded a contract involving 12 industrial and academic organizations from six nations of the EC, for the development of standards for data exchange between CAD programs, finite element programs, and dynamic experimental systems. The project, CAD\*I (a subset of STEP, in ASCII), is also concerned with the design and development of software interfaces for proving the feasibility of the standards. The partners have successfully exchanged CAD and FE modes. The work has been accomplished with the International Standards Organization, which is working on the STEP/PDES standards, and the two organizations have exchanged many ideas.

Arabshahi, University of Leeds, presented a different perspective of FEA. Arabshahi's paper, "An Application of Systems Analysis to Engineering Practice: Finite Ele-

ment Analysis from Solid Models," laid out the process of FEA from a systems point of view. Basically, they tried to get a reasonable representation of what goes on in the analyst's mind using as a starting point the solid model representation of the component to be analyzed. For this purpose, the structured analysis and design technique was used as it is particularly well suited to the documentation of so-called soft systems and is principally used for activity modeling. The authors developed a model that distinguishes between different specific activities and defines the context in which the analyst performs the activities. They believe it can be used to explore the role of QA systems, educate, and reduce the vagueness surrounding the idealization process.

Ward et al., SDRC, U.S., presented a paper discussing targeting their adaptive mesh generator to the 200,000 U.S. designers who do not have FEM expertise versus the 20,000 FE analysts who do. Their market research has led to the automation of mesh generation which accounts for (1) the ability to redistribute nodes; (2) automatic element distortion reduction; (3) maintain independence from specific FE formulation, physical problems, and error messages, and (4) sufficient efficiency for interactive purposes. They use both r-refinement; i.e., the number of nodes is held constant, but redistributed more optimally, and h-refinement where the element size is decreased resulting in a more refined mesh in particular areas.

Factors influencing the accuracy of FEA of free vibration of flat plate structures were investigated by Borthwick and Ng, Heriot-Watt University, U.K. The factors include the degree of discretization, both in terms of number and type of element, the number and choice of automatic masters for the reduced system, and the influence of element shape distortion such as aspect ratio, skew, taper, and edge curvature. Recommendations are made regarding the level of discretization and number of masters required for accurate analysis. Their conclusions are what one would expect; i.e., the results of numerical experiments with distorted elements indicate that the accuracy of natural frequency calculations is hardly influenced, except at very high levels of distortion. However, modeshapes are relatively more sensitive, particularly where mesh line does not conform to the boundary of the geometric shape meshed or violate its symmetry.

G. Butline, FEGS, U.K., spoke on "Towards Mechanical Designers Simulation" (because he wanted to impress the importance of establishing automated procedures for FEA in the hands of designers). Butline discussed the demands of simulation; i.e., abstraction, discretization, validation, solution, visualization, and change. Current parallelism is not providing fast throughput, and massive parallelism is needed to move ahead.

Wheeler, Swanson Analysis Systems, U.S., presented more discussion of error analysis in "An Efficient Error

Approximation Technique for Use with Adaptive Meshing." Implementation of the error approximation of Zienkiewicz and Suh in the program ANSYS allows for efficient error approximation, both in magnitude and location. With knowledge of the approximate location and magnitude of the error, an adaptive meshing procedure can be established. This error approximation technique is a significant advancement in applied FE technology.

Errors in stresses caused by transition meshes was addressed by Armstrong, Queens University of Belfast, U.K., in "Performance of Transition Meshes." The element distortion and the nature of loading as well as the presence of constraint equations was taken into account. An algebraic approach that utilized analytical expressions for the error in stress fields provided an accurate method of measuring the errors in the various meshes and consequently allowed a comparison to be made of the performance of the different meshes. The performance of the mesh incorporating constraint equations compared favorably with the other meshes.

Shannon, Queen's University of Belfast, also addressed the errors in transition meshes in "A Semi-Automatic Transition Mesh Generator Utilizing Constraint Equations." Transition meshes usually do not perform as well as a regular mesh because they contain triangular or distorted quadrilateral elements. An alternative technique to maintain connectivity between regions of different element density is to use multipoint constrain equations. This paper presented a two-dimensional (2-D) semiautomatic mesh generator that uses constraint equations to provide transition in mesh density and can produce very acceptable transition meshes. The quality of elements produced is generally better than those obtained from conventional transition mesh generators, and the number of elements used to accomplish a given transition is less. The author did not mention any problem that would occur with the increased bandwidth of the resulting assembled stiffness matrix.

In a parallel topic, Schiermeier, Noetic Technologies, U.S., discussed his research into "Implementation of P-version Shell Elements into Solid Elasticity Framework." Schiermeier had several objectives: (1) the shell and solid formulations must be compatible, so that shell and solid elements may be joined in a straightforward manner; (2) there should be an hierarchy of shell theories so that in the limit, the shell theory becomes identical to the solid; and (3) there should be QA procedures so that the validity of the results can be determined. This is especially important since with shell elements there may be errors of idealization as well as errors of discretization. Two examples were presented to demonstrate the quality control procedures for p-version shell elements for displacements, stress, and other quantities.

P. Bergan, A.S. Veritas Research, Norway, talked on "The Individual Element Test: A Basis for Checking and

Deriving Elements." Bergan discussed the concept of acceptance tests for FE through establishing explicit requirements that the stiffness matrix must fulfill. This may be done through the individual element test, which is a set of linear constraints that an element must satisfy identically in order to converge. This concept has been extended to a nontraditional way of formulating FE, denoted the free formulation. This method allows for using nonconforming displacement functions as well as tuning of the energy of an element, and it forms the basis for new classes of elements. Current tests are a-posteriori, proposed test is a-priori and can be built into the element formulation as suggested by Zienkiewicz in the opening lecture. The paper gives examples of such elements for membranes, plates, shells, and solids.

Hinton, University College, Swansea, U.K., report the result of the NAFEMS Nonlinear Working Group in "Fundamental Elasto-Plastic Finite Element Benchmarks." One of the products of the NAFEMS Nonlinear Working Group is the specification of a set of fundamental benchmark tests for elasto-plasticity. The tests involve very simple geometric specimens in 2-D plane stress and strain, axisymmetry, and three dimensions. Loading is by prescribed displacement over all the degrees of freedom so that the resulting equilibrium solution is well-posed, and so the tests concentrate on the constitutive models: geometric nonlinearities (rate and temperature effect are excluded). Different hardening models are considered, as perfect plasticity, isotropic, and kinematic hardening.

P. Maserati, CISE Tecnologie, Italy, presented another nonlinear benchmark, "Theoretical and Experimental Benchmark Problems for FEM Analysis of Nonlinear 3-D Structures." (The paper was read by a colleague, Ms. Marishi.) The paper did not pretend to provide a complete and exhaustive collection of benchmark problems for testing a nonlinear structural computer code, but was aimed at presenting numerical and experimental results that can both help to improve the reliability of FEM code and be good training for a specialized user in industry. Puck-2 was the code used for the static and dynamic nonlinear analysis for the 3-D slender structures. Again, there was considerable discussion from the floor on whether experimental benchmarks are a reliable litmus test for these purposes of standardization and QA.

Whereas the previous paper looked at nonlinearities in slender structures, the paper by N. Knowles, of Atkins Engineering Sciences, U.K., dealt with "Benchmark Requirements for the Nonlinear Behavior of Beams and Shells." These structural forms are particularly sensitive to geometrical changes and hence, attention is concentrated principally on geometrical nonlinearities. However, material nonlinearities are not excluded. The author begins with several very well thoughtout objectives and tries to apply them to the general requirements for a

good benchmark. For the beams, the arguments work well; but for shells, as the author acknowledges, there is yet to be a universally reliable, robust, accurate, and efficient shell element to be developed, even for linear applications. But the deficiencies of current elements and the difficulties in overcoming them are reasonably well understood.

M. Smith, W. Atkins Engineering Sciences, U.K., presented "Experiences Running Nonlinear Benchmark Tests Using ASAS-NL." Smith commented on three sets of benchmark tests specific to nonlinear analysis published by NAFEMS. The tests cover elasto-plastic material behavior, solution procedures for geometric nonlinearity, and geometrically nonlinear beams and axisymmetric shells. The following aspects of these tests are reported: educational content, clarity of definition of the tests and target values; resources required to carry out the tests, comparison of ASAS-NL results with target values, and suitability of the tests as benchmarks.

A second paper by Afzali, CETIM, France, "3-D Linear Static Tests for Beams, Plates and Shells, Proposed by French Committee, VPCS," presents the results of one of the VPCS group of the SFM, that is in charge of preparing tests for linear static analysis of beams, plates, and shells. The motivation and the criteria used for the choice of the tests were discussed. The objectives of the VPCS is to provide a handbook in which the tests proposed in different areas are related to the industrial applications.

G. Davies, Imperial College, U.K., presented the last invited paper, "Is NAFEMS Hitting the Right Target?" In retrospect, this paper probably should have been the first invited paper since the author did an excellent job of providing a historical background of the FE method and NAFEMS. Davies proposed that compilation of FE mistakes be tabulated so they would not be repeated but was enough of a realist to know that would never happen. He remarked that the biggest fringe benefit from NAFEMS

has been the educational aspects. Finally, he recommended that NAFEMS now turn to standards rather than just information. Standards of QA are being addressed, once FE developers are aware that 1992 means harmonization of standards in the EC and is going to happen in information technology.

Levesque, Electricite de France, France, presented "Tests of Reference for Dynamics Analysis in the Handbook *Validation of Structural Analysis Software*." In a QA organization, the global validation of engineering software is a deterministic step. The major difficulty in establishing QA procedures is to collect a set of representative tests. To increase the efficiency of computer codes, French developers and users decided to merge experiences of several industries and researchers to collect and validate reference tests in a handbook. The paper describes the methodology used for the definition of the handbook.

J. Maguire presented "The NAFEMS Forced Vibration Benchmarks." The tests cover beam, thin-shell and thick-shell element assemblies subject to harmonic, periodic, transient, and random loading. The work was performed under the direction of the Dynamics Working Group. Only linear, elastic, isotropic, initially stress-free assemblies are considered and attention is focused on the most popular types of FE in commercial use. The tests are for three cases-deep simply supported beam, simply supported thin square plate, and simply supported thick square plate.

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## The 16th Annual International Symposium on Computer Architecture

by Mr. Ashok Singhal, Computer Science Division, University of California, Berkeley.

### Overview

The International Symposium on Computer Architecture (ISCA) is widely considered the primary conference for computer architects. The papers presented each year at the conference are usually indicative of both the state-

of-the-art in computer architecture research and the problems that the professional community considers important to solve. The ISCA held in Jerusalem, May 28 through June 1, 1989, was no exception. This report is my assessment of the important advances revealed by speak-

ers at ISCA 1989 and of the major issues now being addressed by the research community.

Since the papers were presented in two parallel sessions, it was only possible for me to attend half the presentations. My coverage of the presentations that I did not attend is based on the papers in the symposium Proceedings and conversations with the authors and other attendees.

I will first outline the broad trends that were apparent in the symposium. Next, I will focus on specific important developments in all aspects of computer architecture that were presented, emphasizing those developments that I consider significant with respect to my own research on high performance architectures for Prolog. Finally, I will summarize my experience at ISCA 1989.

## Broad Trends

Computer architecture is driven on one hand by requirements of languages and applications, and on the other by the availability of new technology. John A. Darringer, IBM Research, addressed mainly the latter aspect in the opening address, "Trends in Technology and Systems," in which he discussed promising new technologies that are likely to find applications in computer designs of the future. Darringer sees X-ray lithography as an inevitable advancement in integrated circuit process technology because of advantages such as smaller feature sizes and insensitivity to dust particles. New resist materials and masks for X-ray lithography are being developed at Brookhaven National Laboratories. For mass storage, while current magnetic storage densities are 30 to 40 Mbits/sq.in., Darringer believes that 1000 Mbits/sq.in. will be achieved by 1995. The trend will be towards smaller disks used as building blocks with error detection and correction. One can expect a variety of disk architectures to emerge in the next few years. Darringer sees very interesting potential application in mass storage for the recently developed Scanning Tunneling Microscopy, which has sufficient resolution to observe atoms on the surface of a material. With suitable modifications, the technique could be used to store data at a molecular or atomic level, resulting in much greater densities than is possible with any other known technology. The dominant trend in systems has been parallelism. There can be no doubt about its success for many special purpose applications. Several parallel systems are up and running with multi-threaded operating systems such as Mach and we can expect the research in general purpose parallel systems to expand significantly in the next few years.

Michael W. Blasgen, IBM Research, delivered the keynote address, "Evolution to Post-RISC Architecture," in which he dealt with parallelism within each processor. Blasgen sees the *RISC era* as a simplification and consolidation of older ideas rather than the development of any

important new ones. He believes that the *Post-RISC era* will exploit instruction level parallelism with super-scalar architectures, and that all successful future architectures will be developed in an environment of close consultation between the architects, compiler writers, and other programmers.

The most obvious trend that I observed at the conference was the growing importance of cache memories. Of the 46 papers presented, four were about uniprocessor caches, six were about cache coherence and synchronization, and four dealt primarily with instruction caches (instruction fetching). The trend in uniprocessor caches is towards multilevel caches since small, on-chip caches have now become feasible. In multiprocessor systems, cache coherence protocols are being developed for multiple bus architectures so that shared memory systems will no longer be limited to only a few (10 to 30) processors by a single bus.

## Uniprocessor and Multiprocessor Caches

Several shared memory multiprocessors are now available. Many programmers believe that shared memory is the best of the available paradigms. However, these multiprocessors are limited to only a few processors by a single bus. These processors usually have caches that maintain coherence using a "snooping" protocol. The performance of the single bus multiprocessor can be optimized by selecting the right kind of snooping protocol based on extensive cache simulations as demonstrated by Eggers and Katz in "Evaluating the Performance of Four Snooping Cache Coherence Protocols." However, the performance differences between various well-known "snooping" protocols is relatively small and several researchers have realized that any further significant improvements will require a multiple bus architecture for which current "snooping" protocols do not work. In "Multilevel Shared Caching Techniques for Scalability in VMP-MC," Cheriton, Goosen, and Boyle of Stanford University describe the memory system of the VMP-MC. The memory system is based on a hierarchy of shared caches, ranging from on-chip caches to board level caches connected by buses to a high speed fiber optic ring. The consistency mechanism is hierarchically structured and directory based. It is interesting to note that combinations of "snooping" and directory-based coherence protocols for multiple bus architectures have also been proposed in other forums by Jim Goodman, University of Wisconsin, Madison, and Mike Carlton, University of California, Berkeley. The authors report that parts of the VMP-MC system are working and other parts are being designed or constructed. When it is finally completed, the architecture community will find that there is much to learn from the VMP-MC. Goto, Matsumoto, and Tick, ICOT, Japan, describe the "Design and Performance of a

Coherent Cache for Parallel Logic Programming Architectures." Their measurements will prove useful in designing caches for our own Prolog machines at the University of California, Berkeley.

With the increase of static code and dynamic instruction bandwidth in current RISC processors, instruction fetching (and caching) has emerged as an important research topic. Following the current trend towards shifting complexity to the compiler from the hardware whenever possible, Hwu, Conte, and Chang, University of Illinois, suggest in "Comparing Software and Hardware Schemes for Reducing the Cost of Branches," that compilers can rearrange code, based on dynamic traces, to reduce the cost of branches. They show that the software scheme has better performance than hardware schemes based on branch target buffers that have greater hardware complexity. In another paper, "Achieving High Instruction Cache Performance with an Optimizing Compiler," Hwu and Chang describe algorithms used in their IMPACT-1 compiler to rearrange code (again, based on dynamic traces) in order to increase spatial locality of code references and thus increase instruction cache performance. The primary research contribution of Steenkiste's, Stanford University, paper, "The Impact of Code Density on Instruction Cache Performance," is a methodology to estimate cache performance of various architectures based on measurements for a single architecture and code densities for the architectures. This is potentially a very useful tool for computer architects. Steenkiste has used the technique to show that even relatively moderate changes in code density can have large impact on instruction cache performance.

### Pipelined and Parallel Architectures

Murakami, et al., Kyushu University, Japan, described their Single Instruction Stream/Multiple Instruction Pipelining (SIMP) processor. The SIMP is not an instruction set architecture, but rather a high performance vehicle for implementing several different architectures. The SIMP resembles the high-performance substrate microarchitecture of Yale Patt, University of Michigan, and consists of multiple identical pipelines that execute one instruction per cycle each. At first glance, SIMP may resemble the VLIW but it is actually quite different because, unlike the VLIW, the number of pipelines is transparent to the compiler; the hardware handles all the data and control dependencies. They measure a speedup of up to 2.72 over a single instruction pipe using four instruction pipes. The most attractive feature of SIMP is that the number of pipelines is transparent to the compiler. Therefore, the code can be binary compatible across versions of the processor that have different numbers of pipelines.

There were several very interesting papers in the session on parallel architectures. Nikhil and Arvind described how a data flow processor could be used to execute von Neumann style programs in which parallelism is exploited by multiple threads specified by "fork" and "join" constructs. Weber and Gupta described the architecture of a processor that supports a small number of hardware contexts and fast context switching so that processor utilization can be increased by switching context at cache misses or write-hit to shared data. In large networks of processors, the latencies involved in cache misses or writes to shared data could be long. A question from the audience (Jim Goodman, University of Wisconsin, Madison) raised an important issue related to this work: is it better to have more simple processors with single contexts and lower utilization (because they stall on cache misses and network accesses), or to have fewer, more complicated processors that have higher utilization because they have multiple contexts and faster context switching? To the best of my knowledge, this is an open research question that will become increasingly important as large-scale multiprocessors evolve.

### Prolog Architectures

This year, there was one session devoted to Prolog architectures. Since my research is on high performance Prolog architectures, and since I presented a paper in this session, it was of special interest to me. Benker, et al., ECRC, Federal Republic of Germany, described "KCM: A Knowledge Crunching Machine" and its Prolog performance. The KCM, like most other Prolog machines, is based on the Warren Abstract Machine. The KCM is designed as a backend processor with its own memory system and local bus, connected to a UNIX host through communication memory. The machine is constructed with ASICs and off-the-shelf TTL and complementary metal oxide semiconductor (CMOS) parts with a cycle time of 80 nsec. The KCM achieves a performance of between 222 and 766 kilo logical inferences per second, depending on the benchmark, or about 7.85 times the performance of Quintus Prolog (one of the fastest commercial Prolog systems) running on a Sun 3/280. The main features are a 64-bit word for both data and instructions, and an instruction encoding that allows two register moves per cycle. The KCM is a microcoded machine and its special support for unification includes a 16-way address calculator based on the type tags of two operands. Morioka, Yamaguchi, and Bandoh, Hitachi Research Laboratories, discussed the design alternatives they considered for the cache in their Integrated Prolog Processor (IPP). They chose a store-through cache with a multistage write buffer and an interleaved memory. Wong and Williams described "A Type Driven Hardware Engine for Prolog Clause Retrieval Over a Large Knowl-

edge Base" called CLARE. The CLARE uses superimposed code words with mask bits to select candidate clauses from a large set of clauses on disk to satisfy a given query. These filtered clauses are then sent to Prolog software system that completes the computation for the query. In "A High Performance Prolog Processor with Multiple Function Units," I described the Parallel Unification Machine (PLUM). The PLUM overlaps execution of bookkeeping operations with unification in Prolog by executing them on multiple function units. Unification is also speeded up by exploiting parallel unification using multiple unification units. A speedup can be achieved of approximately 4 over a sequential system.

While Prolog processors have yet to become commercially successful, their performance has improved significantly because of better processor designs and optimizing compilers. Even though commercial general purpose processors have faster clocks since they use newer technologies, special purpose Prolog processors offer higher performance because of special architectural support.

## Performance Evaluation

The communication bandwidth of a multiprocessor can be increased by either increasing the width of the bus, or by increasing the number of buses. Intuitively, multiple buses should have better performance for the same number of data lines because they are more flexible than a single bus. Hopper, Jones, and Lioupis, Olivetti Research, U.K., show that this is indeed true by comparing the performance of a wide bus (128 bits wide), 2 buses (each 64 bits wide), and 4 buses (each 32 bits wide) connecting 16 processors. However, the performance differences were not as large as I would have expected, and it would seem that the single wide bus would still be preferable to the multiple bus architectures because of simplicity and cost. No measurements were shown for a system with more than 16 processors, but I would guess that the same conclusions would not be valid for larger systems.

Annaratone, Pommerel, and Ruhl, Swiss Federal Institute of Technology, investigated the tradeoff between performance and channel communication performance in distributed memory parallel processors, in particular processors connected in a torus mesh. They identify an ideal range for the parameter  $q$  which is the ratio of the time for a processing element (PE) to receive or send a double precision quantity from a neighboring PE to the time to perform a double precision multiply-add operation. They conclude that  $q$  should be smaller than 8, but too small a  $q$ ; e.g., 0.5 for iWARP, could mean an overdesigned communication channel.

## Simulation Systems

Since logic simulation of large digital designs is very time consuming, it is a good candidate for parallel execution. However, because of the extremely fine grain size of the parallel task, the irregular nature of interconnection and high volume of communication, it is difficult to get good speedups. Kravitz, Bryant, and Rutenbar CMU, describe compilation tools to map the logic simulation problem onto massively parallel SIMD architectures such as the Connection Machine. Unlike simulators on sequential processors, the COSMOS simulator that the authors describe is not event-driven. While an event-driven simulator can eliminate some extra computation, it also makes it harder to extract parallelism.

Fukazawa, Kimura, and Tomizawa, NIT, Japan, describe "R256: A Research Parallel Processor for Scientific Computation." They contend that many currently available parallel processors do not have the communication bandwidth required to support device simulation computations. The R256 is a room-sized machine that is composed of 16x16 processing elements connected by distributed parallel network that can achieve 2 GB/s data transfer rate and 500 MFLOPS computation rate on semiconductor device simulations. The processors are VLSI chips but the rest of the machine is built using conventional TTL ICs. The most interesting feature of the R256 is the high bandwidth distributed parallel network, which requires fewer communication steps than either array processors or hypercube interconnects.

## Summary

Of all the aspects of computer architecture discussed at ISCA 1989, caches got the most attention. Since programmers seem to prefer the shared-memory paradigm of multiprocessors, computer architects are studying cache coherence protocols. Protocols based on a single bus have been used for some time. Research on cache coherence protocols for other interconnects is now in progress at several sites around the world. The trend in processor design is to expose more of the hardware to optimizing compilers. Some researchers also propose exposing the memory hierarchy to the compiler; code reordering by the compiler can improve conditional branching and code locality in instruction caches. Other topics discussed were pipelined and parallel processors (including dataflow), mapping algorithms, networks, Prolog architectures, performance evaluation, logic simulation systems, and memory systems. One important topic that was conspicuous by its absence was input/output architectures.

# CONDENSED-MATTER PHYSICS

## 9th General Meeting of the Condensed-Matter Division of the European Physical Society

by Dean L. Mitchell, the Liaison Scientist for Solid-State Physics in Europe and the Middle East for the Office of Naval Research European Office.

On 6-9 March, 1989, the Condensed-Matter Division (CMD) of the European Physical Society met in Nice, France. With attendance at about 600, it is the same size as the U.K.'s annual solid-state meeting and is one-third the size of the corresponding meeting for the German Physical Society. The CMD meeting is, at present, considered to be an optional supplement to national meetings. However, the recent upward trend in attendance at this meeting indicates that it is becoming more widely recognized and may ultimately become *the* European forum for condensed-matter physics in the same sense that the March meeting of the American Physical Society (APS) is *the* meeting in the U.S. for condensed-matter physics and related material sciences.

The first three mornings of the meeting opened with plenary sessions that included nine talks. The topics included: High  $T_c$  Superconductors by G. Deutscher; Heavy Fermions by F. Steglich; Metallic Clusters by W.D. Knight; Neural Networks by B. Derrida; Instabilities and Turbulence by A. Libchaber; Quasicrystals by D. Gratias, and Magnetic Metallic Multilayers by J.J. Rhyne. The plenary sessions were followed by poster sessions which included a total of 438 contributed papers (see Table 1).

Table 1. Contributed Topics

Theme	Number
Surfaces and interfaces	64
Semiconductors	72
Superconductors	91
Metals and alloys	82
Disorder	68
Tunneling and other	61

The afternoons and the fourth morning were devoted to invited talks organized in three parallel sessions. The

invited talks were on topics of current interest, both basic and applied. Superconductivity, including organic and heavy fermion systems, drew 16 papers; semiconductors also had 16 papers with emphasis on surfaces, interfaces, and heterojunctions. The latter included work on the one- and two-dimensional (2-D) electron gas systems and on strained-layer heterojunctions. Fluids, including studies of instabilities, phase transitions, surface wetting, gels, and glasses were represented by 12 papers, while fractals, localization, and disorder phenomena were covered in 6 papers. The remaining 22 papers were concerned with a variety of topics including bio-medicine, polymers, materials processing, and new device technologies.

G. Deutscher, Tel Aviv University, Israel, in his plenary talk, reviewed recent infrared and tunneling experiments bearing on the magnitude of the superconducting energy gap in rare-earth/copper-oxide superconductors with high critical temperatures (high  $T_c$ ). Using generalized arguments based on Ginzburg-Landau theory, he concluded that the energy gap exists over the entire Brillouin zone but that the correlation lengths are anisotropic. The correlation lengths were estimated to be 5-15 Angstroms in the ab crystallographic plane and 2-5 Angstroms in the perpendicular direction, along the c axis.

B. Derrida, Service de Physique Theoretique CEN, Saclay, France, reviewed the application of spin-glass models to neural-network simulation. Derrida traced the evolution of the models and the relation to associative memories via the Hopfield model. Then he discussed the dynamics of randomized spins interacting with symmetrical coupling. The associative memory patterns were defined in terms of the attractors in phase space for the coupled nonlinear dynamical equations. The main emphasis of the talk was devoted to the dynamics of spin-glass networks with asymmetric interactions which, it was argued, may be more realistic for simulation of biological neural networks. The dynamical properties for a class of dilute asymmetric networks were calculated analytically.

Many of the properties were similar to those previously derived for symmetric networks. However, in some instances, the asymmetric case is more tractable for nonequilibrium cases than its symmetric cousin. It also exhibits behavior not present for the symmetric case; e.g., chaos.

The invited papers covered a diversity of topics not all of which will be reviewed here. My overall impression of the meeting was that the invited talks were on a par with those at the March APS meeting in the U.S. both in terms of topicality and in terms of the range of topics covered. The following résumés are for those talks that I found to be particularly interesting or significant.

The phenomenology for quasi-one-dimensional transport and magnetotransport of ballistic electrons confined in quasi-2-D quantum wells or surface inversion layers was further developed in the talks given by C.W.J. Beenakker, Philip's Research Laboratories, Eindhoven, the Netherlands, and by B.J. van Wees, Delft University of Technology, the Netherlands. Beenakker drew on the analogy with magnetic field induced electron focusing as explained for pure metals by Sharvin in 1965. In this model, the spectral features observed in the magneto transport result from mode interference of the electrons in an "electron waveguide." In a sense, the system defines a hot electron spectrometer. The talk by van Wees, a sometime collaborator with Beenakker, drew on similar phenomenology to derive the variation of the zero-field conductance for narrow constrictions. The constrictions were determined by closely separated side gate electrodes placed on the surface. The width of the constriction was varied by changing the gate voltage. For effective widths smaller than the Fermi wavelength and for very long mean-free-paths, the conductance had features in common with the quantum Hall effect; i.e., the conductance was quantized in units of  $2e^2/h$ . The value of the average conductance, which he defined as the "Sharvin" conductance, was shown to scale with the width as expected for this model.

Diffusion in porous media was discussed by J. Feder, University of Oslo, Norway. He developed a model for displacement of one fluid by another based on extensions of the Darcy equation, which originally was proposed for displacement of a single fluid. An additional constraint was imposed by Poisson's equation. The experiments were conducted in 2-D porous media with glycerol injected at the center of the plate. The wavefront developed fractal characteristics with erose boundaries consistent with the scaling model he derived that was based on Koch trees. The fractal dimension of the model calculation was 1.64 in agreement with the experiments. These results indicate that models of oil recovery cannot be expected to give quantitative results unless the fractal nature of the diffusion front is taken into account.

Another study involving fractals was carried out by R. Vacher, the Université des Sciences et Techniques, Languedoc, France. Silica aerogels were prepared with porosities in the range of 80-99 percent. Small angle neutron scattering studies indicated that the aerogels were comprised of small dense blobs of mean radius "a" connected in a fractal network which extended outward to the correlation length "l". The fractal dimension was determined as  $D = 2.5$ . The structures of the aerogels determined here are very similar to those of carbonaceous soots, which have been studied previously. Brillouin and Raman scattering studies were carried out over a wide frequency range. The measured cross sections exhibited the expected crossover for vibrational modes from phonon to fractal behavior as the frequency increased. The crossover was in the expected range. Also, self-similar scaling was observed in the fractal regime.

Other model calculations of fractal behavior were reported by R. Dekeyser, A. Maritan, and A. Stella at the Katholieke Universiteit Leuven, Belgium, who have applied renormalization group techniques to analytically determine the dynamical properties of deterministic fractals. In another numerical study, L. de Arcangelis, the Service de Physique Theoretique CEN, Saclay, France, discussed a fractal model for fracture using a random fuse network to simulate the fracture process. The results of the simulation appeared to be invariant with respect to the various distributions of disorder and fuse thresholds which were assumed.

Synchrotron radiation has become widely accepted in Europe for a wide variety of structural and spectroscopic measurements of biomaterials, structural materials, molecular systems, and solid state or condensed-matter systems. At the CMD meeting, reports were given on studies of clean semiconductor surfaces carried out by M. Sauvage-Simkin at the Laboratoire pour l'Utilisation du Rayonnement Électromagnétique (LURE) synchrotron source, Orsay, France; kinetic studies of proteins and viruses by H.J. Hadju, Oxford University, U.K.; and, circular polarization studies of magnetic solids carried out by G. Schultz, the Technical University of Munich, Garching, Federal Republic of Germany (FRG). The latter experiments were carried out at the DORIS II storage ring located at the HASEY laboratory, Hamburg, FRG. The Extended X-Ray Absorption Fine Structure (EXAFS) spectra as well X-ray Absorption near Edge Structure (VANES) spectra for iron, cobalt, and nickel (as well as rare earth impurities in iron) were measured using circularly polarized radiation from the DORIS synchrotron source. Circular polarizations of 80 percent were attained for photon energies in the range 5-20 eV. In the near-edge spectra, the absorption coefficient reflected the spin-dependent density-of-states near the Fermi level. The experimental results for iron agreed with calculations based on the known band structure.

However, the results for cobalt and nickel did not agree with band structure calculations. No explanation was provided. Experiments also were carried out on 3d, 4f, and 5d impurities in iron matrices.

A summary of research on the processing and fabrication of polymeric devices at the Cavendish Laboratory, Cambridge, U.K., was given by R. Friend. The program is directed toward the development of processing techniques for fabricating electronic device components.

Chemically doped polyacetylene has been prepared with conductivities within a factor four of the conductivity of copper at room temperature. Undoped, it is a semiconductor. In order to fabricate devices, first a precursor

p-type base structure was applied to a silicon substrate by spinning. Next, metal electrodes were evaporated to provide either Ohmic or blocking contacts. Silicon or silicon-oxide were used for substrates and insulating layers. To date, diodes and metal-insulator-semiconductor-field-effect-transistors have been fabricated that have reasonable device characteristics for low-frequency operation on the order of 100 Hz. There do not appear to be any adverse effects from surface states. The current studies are directed to determining the physical and processing variables limiting the performance characteristics of polyethylene devices.

## MATERIALS SCIENCE

### Lasers in Surface Science: A Topical Conference in Trieste

by Milton Kabler, physicist in the Condensed Matter and Radiation Sciences Division, Naval Research Laboratory, Washington, D.C.

#### Introduction

Although Trieste, a midsized port city on the Adriatic Sea near Austria and Yugoslavia, is historically only recently Italian, and is being particularly well treated by the Italian government in regard to support for science. Not only are the International Centre for Theoretical Physics (ICTP), the International School for Advanced Studies, and Trieste University all in or near the city, but it also will be the site of a major new Italian synchrotron radiation source (somewhat similar to the Advanced Light Source being built at Berkeley) and complementary to the larger European Synchrotron Radiation Facility under construction at Grenoble.

In keeping with the character of the place, each summer Trieste becomes the location of a series of topical conferences, the Adriatico Research Conferences, which are managed by the ICTP and take place in a modern, motel-type facility at Miramare, 7 km north of Trieste. These conferences are purposely kept small, generally fewer than 100 participants, and are reminiscent of Gordon Conferences in the U.S. This year's topics included Spin and Polarization Dynamics in Nuclear and Particle Physics, Unoccupied Electronic States, Computer Simulation Techniques for the Study of Microscopic Phenomena, Theoretical Understanding of High T<sub>c</sub> Superconductors, and Frontier Sources for Frontier

Spectroscopy. This report discusses the Application of Lasers in Surface Science, August 23-27, 1988, which was organized by Peter Andresen, Max Planck Institute, Göttingen, Federal Republic of Germany (FRG); Hajo Freund, University of Bochum, FRG; and Ward Plummer, University of Pennsylvania. Evidently, it was the first international conference under the general topic of lasers in surface science, which is by any measure a thriving area.

Lasers can be powerful tools for surface science as well as a good organizing theme for a small conference. The attendees represented several "weakly coupled" areas of surface science and this factor, along with the currency and high quality of the science, provided a very stimulating week. But it remains to be seen whether the conference will be one of a kind or whether it will take on a life of its own. The general tenor concerned surface more than laser, and most sessions were near what one might consider the present mainstream of surface science. This synopsis will touch on a representative sample of the presentations, according to my impressions and interests. Proceedings of the conference are not available.

#### Photodesorption

Professor G. Ertl, Fritz Haber Institute, Berlin, gave the keynote lecture and pointed out that three distinct

groups of laser users could readily be identified. The groups are

- People who use lasers as probes of surface properties in various spectroscopic experiments, second-harmonic generation, and two-photon photoemission
- Those who are concerned with surface chemistry including desorption, etching, and deposition
- Those who study molecule-surface interaction dynamics using lasers to excite and interrogate specific states.

Most of the subsequent papers came from the first two groups, while Ertl concentrated on the second and third. He emphasized a fundamental question: Is a given laser-induced process initiated entirely by heat from the absorbed light; or by electronic excitation that creates electrons, holes, excitons, plasmons, or direct excitation of bonds; or by both? That is, what are the relative contributions of thermal and photochemical processes? Ertl offered three operational criteria for proof that a given process is photochemical.

- (1) Threshold or resonant behavior must characterize the excitation spectrum for the process; this is not sufficient by itself, since resonant heating can occur where an electronic transition simply acts as an antenna.
- (2) The process must be selective; e.g., different adsorbate states must respond differently at the same temperature.
- (3) The kinetic energy distributions of final states must show a nonthermal component.

These criteria can be applied to particle as well as photon excitation, with proper flexibility in using the first criterion.

Ertl gave several current examples to illustrate these points. One was an experiment by W. Hoheisel et al., University of Heidelberg, which showed that low-intensity laser excitation resonant with the plasmon absorption of small ( $\sim 50$  nm) sodium particles caused desorption of sodium atoms with kinetic energies an appreciable fraction of the photon energy, the conclusion being that a plasmon can decay by breaking free an atom at the otherwise cool surface. Another example was ultraviolet excimer-laser-induced desorption of NO from a nickel surface done by Ertl's group in collaboration with scientists from Göttingen and Bochum. Using laser-induced fluorescence (LIF), they obtained rotational and vibrational state distributions for the desorbed NO molecules. Both thermal and nonthermal components were observed in the kinetic energy distributions and, for the nonthermal component, the rotational and vibrational distributions were also nonthermal. In order to observe photodesorption, it was necessary to convert a thin layer of the nickel substrate to nonmetallic oxide, presumably to mitigate the competing de-excitation channels involv-

ing electron and hole creation in the metal. This quenching ability of metal substrates is well known and was emphasized by later speakers.

Looking toward the future from his present perspective, Ertl foresees trends toward using faster laser pulses for better temporal resolution, using laser excitation with scanning tunneling microscopy, a continuing emphasis on nonthermal processes, and an increasing number of state-selective studies of molecule-surface interactions. By the end of the conference, his prognosis looked as good as any.

T.F. George, State University of New York, Buffalo, gave the theoretical overview. He claimed the existence of a broad array of recent advances more or less congruent with Ertl's outline, although he acknowledged that theory is generally lagging behind experiment. For details, see the 1987 issue of the *Journal of the Optical Society of America* which George edited. An apt example of new theory was provided by P. Nordlander, Vanderbilt University, Nashville, who discussed excited adsorbate levels near metal surfaces, a fundamental problem. As an excited, hydrogenlike atom approaches the surface, the electron becomes able to tunnel into the metal, and the energy level shifts and broadens. Nordlander used density functional theory to calculate the energies and widths of the lowest excited levels of hydrogen and the alkalis as a function of distance from aluminum and sodium surfaces. When both the image potential and the s-p hybridization of the excited orbital were taken into account, calculations gave linewidths (lifetimes) in agreement with experiment, a mark missed by previous theories.

H. Zacharias, University of Bielefeld, FRG, presented a paper on state selective desorption. He observed that the occupancies of specific vibrational and rotational states of almost all diatomic and many polyatomic molecules can now be measured directly using tunable dye lasers. This can be done using either LIF spectroscopy or by resonant multiphoton ionization spectroscopy. Thus, the vibrational and rotational state distributions of molecules desorbing or scattering from a surface can be determined. Among the examples was the reactive, thermally activated desorption of  $H_2$  and  $D_2$  from copper and palladium. Here the rotational distributions have been observed to be "cooler" than the substrate, while vibrational distributions are generally "hotter" than the surface. Although these effects are well established, and one can envision model desorption processes that behave in similar ways, their true origins in specific experiments remain unknown.

Reflecting the surface scientist's longstanding fascination with simple diatomic adsorbates such as CO and NO, there were four consecutive papers on laser-induced desorption of NO. K. Kolasinski, Stanford University, and L. Richter, National Bureau of Standards, discussed desorption from Pt(111); E. Hasselbrink, Fritz Haber In-

stitute, FRG, from Pd(111); and S. Sibener, University of Chicago, from Ag(111). As noted above, the kinetic energy distributions of photodesorbed NO generally comprise both a thermal and a nonthermal channel. In all four papers, state-selective spectroscopy showed that rotational distributions are also strongly nonthermal. Evidently, the electronic excitation, whatever its nature, that detaches NO from the surface can also transfer angular momentum, which shows up in some rotational states but not others. Surprisingly, Kolasinski showed that this can also be true for the thermal channel. His measured rotational distribution was polarized in favor of rotation *in the plane of the surface* at high values of angular momentum. How can this happen, particularly because NO adsorbs with its axis *perpendicular* to the surface? Kolasinski speculated on the possible role of an as yet unobserved, weakly bound intermediate state, but the audience was virtually scrambling for plausible mechanisms. The question is open. Richter's model for nonthermal photodesorption also proved thought provoking. His state-selective data included dependences on the desorbing photon energy (Nd:YAG and harmonics) which were shown to support a nonthermal mechanism; in a sense, the NO remembers the energy of the photon which desorbed it. He explained the data in terms of a process involving scattering or transient trapping of a photo-generated hot electron whose energy is resonant with the unoccupied  $2\pi^*$  levels of the adsorbate. Richter showed that this model agrees at least qualitatively with experiment. Indeed, a similar process was suggested previously by Z. Ying and W. Ho to explain photodesorption of NO from silicon. But questions of the size of cross section for such a process as well as the way such a resonant encounter might absorb a neutral NO molecule remained open. From these four papers, it was clear that NO photodesorption will continue to be an active area for a while.

One of the best review talks of the conference was given by D. Menzel, Technical University, Munich, entitled "Photon Stimulated Desorption: What Has Been Learned." He emphasized several general observations, conclusions, and caveats concerning desorption induced by electronic transitions, an alternative title used often enough to have spawned the acronym DIET. Menzel framed his discussion in terms of two contrasting examples, the first a molecular chemisorbate; e.g., CO or NO, on a metal; the second an insulator surface with or without an adsorbate.

Because of the abundance of low-energy excitations, the metal tends to quench any valence excitation in the adsorbate before it can break a bond and cause desorption. For an excitation otherwise favorable for desorption, fast de-excitation by the metal can reduce the desorption probability by several orders of magnitude. However, if this same excitation occurs on an insulator,

there is no fast metallic de-excitation, and the desorption probability can actually be enhanced by secondary band gap excitations in the bulk or at the surface. For metals, when the exciting photons are in the valence region where lasers are most useful, desorption efficiencies are generally very small and one observes many more neutral species than positive ions (negative ions are always rare). This can sometimes be explained by reference to relevant potential curves, among which the ionic states generally lie higher. But for photon energies into the core region, the domain of synchrotron radiation, yields increase (though still small), thresholds begin to appear, and the ratio of ions to neutrals approaches 1. In many cases, one can infer that complex, strongly localized states comprising multiple excitations are dominant in the desorption process. De-excitation channels involving the metal are effective in keeping the desorption yield low. By contrast, desorption yields from insulators such as ionic or rare gas crystals are often enhanced by substrate excitations. For example, excitonic features characteristic of the substrate frequently occur in desorption spectra of insulators. Much remains to be learned about the details of these processes. In later discussions, Menzel made the point that the dependence of photodesorption yield on coverage can be enormous, as can the influence of coadsorbates such as oxygen. Hence, care must be taken in characterizing one's sample and in comparing data sets from different groups.

Approaching the problem through a detailed and realistic theoretical model for fluorine on aluminum, Ph. Avouris, IBM, Yorktown Heights, was able to go much further into the physics of the photodesorption process. He and others had calculated potential curves for different charge states of fluorine using density-functional theory and a jellium model for the metal. Screening was also taken into account, a factor which all previous calculations had neglected. It was found that, in the ground state, the fluorine is a negative ion and is strongly bound to the metal. When the  $F^-$  loses an electron (valence or core), the image potential vanishes and the overall potential becomes repulsive. The now neutral fluorine will desorb if the state is sufficiently long lived, which is the case if the electron lost is a valence electron, but probably not if a core electron. On the other hand, the core hole will decay rapidly via a CVV Auger process, and calculations show that desorption as  $F^+$  can occur. Here screening is crucial in facilitating desorption, because screening charge is transferred from the metal toward the (loosely bound)  $F^+$ , thus greatly decreasing the image potential. The predicted behaviors generally seem consistent with experiment. It was argued that these desorption mechanisms, and particularly the role of screening, can apply to a wide range of systems, including molecular adsorbates and high-dielectric-constant semiconductors.

## Laser-Excited Photoemission

The conference was punctuated at midpoint by a session on two-photon photoemission spectroscopy (2-ph photoelectron spectroscopy [PES]) from surfaces. It has only been within the last 6 years or so that short-pulse photoemission techniques have advanced to the point of yielding reliable, quantitative data. It is now possible to measure energy distributions of photoelectrons originating from normally unoccupied states (states above the Fermi level) with angular resolution as well as with time resolution into the picosecond range. In effect, the technique is the inverse of inverse photoemission; a particular state of interest will be an intermediate state in 2-ph PES but a final state in inverse photoemission. In the review talk, J. Bokor, AT&T Bell Laboratories, Holmdel, New Jersey, stressed the capability of 2-ph PES to provide good resolution in energy, momentum (angle), and time. The price one pays is the formidable combination of source and PES instrumentation that is required. He did not dwell on instrumentation and source technology, but instead emphasized phenomena and conclusions. In fact, this approach was taken by almost every speaker, a circumstance that made the conference particularly agreeable.

Bokor gave an historic description of the field, emphasizing the work of Bensoussan and Moison at CNET, Bagneux; Steinmann and coworkers in Munich; and Long, Williams, and coworkers at the Naval Research Laboratory (NRL), Washington, D.C., as well as Bokor's own group at Holmdel. The range of studies so far includes bulk and surface states in a number of semiconductors, image potential states on several metals, states involving adsorbed oxygen on copper, polaron/soliton excitations in polyacetylene, and excitons in solid rare gases. Examples taken from Bokor's own work included results on the distributions and lifetimes of surface states on cleaved InP and GaAs. Looking to the future, he foresees moves toward using more broadly tunable ultraviolet probes such as free electron lasers, laser-produced plasmas, and synchrotron radiation, and toward the femtosecond time domain. Maturity of the 2-ph PES field is certainly beyond the horizon.

Continuing the session, and fulfilling Bokor's predictions to some degree, R. Schoenlein, MIT, described the first femtosecond 2-ph PES measurements of the lifetime of the  $n = 1$  image-potential state on Ag (100). He and collaborators from General Motors Research Laboratories, Warren, Michigan, used a colliding-pulse, mode-locked, dye laser with a copper-vapor-pumped amplifier. Because the  $n = 1$  state was 0.53 eV below the vacuum level, it was required that ultraviolet be used to populate the state and be used to produce photoemission, a reversal of the normal order in such experiments. Their measured lifetime was between 15 and 35 fs, reflecting the

ease of decay of the state into the metal via Auger processes. Theoretical lifetimes agree with this measurement.

J. Long, NRL, discussed time-resolved measurements of pulsed-laser-induced photovoltages on a variety of silicon (111) surfaces using synchrotron radiation as a probe to measure core level shifts. The magnitude and complex decay of the photovoltages were found to depend on adsorbates, on doping (n- or p-type), and on bulk lifetime. A numerical treatment of the electron and hole diffusion problem was able to reproduce most features of the data. Long noted that values of surface recombination velocities for these surfaces, obtained from the measured decay curves, were generally found to be in the high range (greater than  $10^5$  cm/s), a significant new result.

The first 2-ph PES work on diamond was described by G. Kubiak, Sandia Laboratories, Livermore. Using a pulsed tunable dye laser with harmonic generation and mixing, and with photoelectron angular resolution of  $\pm 1^\circ$ , he was able to map the dispersion of a normally empty surface state high in the band gap on the diamond (111) 2 x 1 surface. Theory had suggested a  $\pi$ -bonded chain reconstruction and a related surface state, in reasonable agreement with the data. Kubiak interpreted his results as confirming the  $\pi$ -bonded chain reconstruction.

A midgap surface state on the cleaved Si(111) 2 x 1 surface was the subject of N. Halas, AT&T Bell Laboratories, Holmdel. The 2-ph PES technique was used here principally to measure the decay of this state, populated either by direct optical transitions or by electrons pumped into the bulk conduction band. An appropriate carrier diffusion and trapping model was developed for comparison. And finally, adding further to the array of surfaces explored in this session, R. Haight, IBM, Yorktown Heights, described an experiment on GaAs(110) which used 2-ph PES to measure a surface intervalley scattering time. Electrons were pumped into the conduction band at the center of the Brillouin zone, from which they scattered into the normally empty surface state associated with the X valley. The measured scattering time was 0.4 ps.

This session gave a good overall view of current activity in 2-ph PES. Its only shortcoming was a lack of first-hand accounts of the considerable European efforts which were, for various reasons, without representation.

## Vibrational States, Surface Reactions

The conference now turned to the vibrational spectroscopy of molecules on surfaces, a field that stands to gain much from the infrared free electron laser (FEL). S. George, Stanford University, described two of the first such experiments using the Mark III IR FEL at Stanford. In one experiment, the spectrum of physisorbed butane on Al<sub>2</sub>O<sub>3</sub> was determined by measuring the desorption yield as a function of wavelength. Since the butane mole-

cules are weakly bound, resonant heating is sufficient to cause desorption. He established that the effect was resonant heating and not state-selective desorption by showing that, for a mixture containing 50 percent deuterated molecules, all molecules came off with equal probabilities when a vibration of either the normal or the deuterated butane was excited. In the second experiment, he measured the surface diffusion coefficients of n-alkanes by resonantly desorbing a well-defined spot and following in real time the refilling of the spot by molecules from the adjacent area. George found that for simple C<sub>3</sub> to C<sub>6</sub> alkanes on ruthenium, the diffusion activation energies E<sub>d</sub> were relatively low, in the 3-5 kcal/mol range, and increased with chain length. There was essentially no coverage dependence, E<sub>d</sub> increased with chain length, and the ratio of E<sub>d</sub> to the desorption energy was approximately constant at 0.3. He is trying to model this result using simple potentials and polarizabilities.

In this session on surface spectroscopy, there were also several papers on surface reactions. E. Fridell, Chalmers University of Technology, Göteborg, described studies of the kinetics of reactions of H<sub>2</sub> and O<sub>2</sub> on platinum at 900-1200 K to form OH and H<sub>2</sub>O. The desorbing OH was detected using LIF. The LIF was used also by a group from the Max Planck Institute for Quantum Optics, Garching, represented by K. Wagemann. The purpose was to detect desorbing CuF molecules formed in a dry etching reaction of molecular or atomic fluorine with Cu(111) at temperatures in the 750-1150 K range. In this case, the vibrational temperature of CuF measured by state-selective fluorescence was comparable to the substrate temperature. Finally, R. Osgood, Columbia University, New York, described work on the oxidation of GaAs which, in contrast to the two previous papers, uses a laser to initiate the reaction on the surface. The greatly enhanced oxidation rates attained during laser irradiation can, at least at low oxygen coverages, be ascribed to electrons and holes formed in the semiconductor which diffuse to the surface and stimulate oxide formation. Laser heating seems to play no role.

### Nonlinear Spectroscopy

The last major topic of the conference was surface nonlinear optical processes. For surface characterization and analysis, the most useful of these appear now to be second harmonic generation (SHG) and sum-frequency generation (SFG), second-order processes which have inherent surface-sensitive components. By contrast, coherent anti-Stokes Raman scattering (CARS) is third order and is not inherently sensitive to the surface. These aspects were reviewed by R. Shen, University of California, Berkeley, who has contributed more than anyone else to the development of the field.

In experiments mentioned thus far, it has been more or less obvious how a laser probe can achieve surface sensitivity. Even though light is absorbed over a depth comparable to or greater than the wavelength; i.e., over many bulk atomic layers, the depth sensitivities are determined by the escape depths of the photoelectrons, ions, and molecules which comprise the secondary particles actually detected. In contrast, SHG is a photon-in, photon-out measurement, and the surface sensitivity comes about in a different way. To be electric-dipole-allowed, SHG and SFG require nonexistence of inversion symmetry. In a centrosymmetric material, it is only at an interface that inversion symmetry is broken. Thus, dipole-allowed SHG and SFG occur only at interfaces. However, there are always higher order bulk contributions; i.e., electric quadrupole and magnetic dipole, and in most measurements the main task is to separate these from the surface contribution. The prototypical SHG experiment is done in reflection.

Shen noted the potential advantages of SHG and SFG: they involve relatively simple experiments, are nondestructive, do not require vacuum, are widely applicable, and are well suited for studies of subpicosecond surface dynamics. As an example of the latter, Shen mentioned a measurement of surface diffusion done by burning a grating through an adsorbate and then measuring the time dependence of the SH as the grating decays by adsorbate diffusion. One disadvantage of SHG is its general lack of molecular selectivity. The reason is that, in the near-infrared and visible, which is the range where one wants to work because detector sensitivities to the SH frequency are high, the resonances are broad and not particularly burdened with information. This disadvantage can be overcome by using SFG with a fixed visible beam along with an infrared beam tunable through the vibrational resonances of the molecule. The vibrational resonances then appear as molecule-specific resonant enhancements in the SF signal. This is another area where the FEL can be expected to prove useful in the future.

An invited paper on the theory of SHG was presented by A. Liebsch, Jülich, FRG. His talk dealt entirely with calculations, again using the jellium model for simple metal surfaces. A time-dependent density functional approach was used to obtain the nonlinear response of the metal to frequencies below the plasma frequency. What happens is that the light generates a shallow SH current or screening field normal to the surface which depends sensitively on the nonlinear screening properties near the surface and which exhibits Friedel density oscillations. Liebsch's calculation showed that this normal damped oscillatory polarization is much larger than simpler theories had suggested and can strongly affect the SHG. Later, K.J. Song, University of Pennsylvania, described experiments that appeared to provide a very satisfying confir-

mation of Liebsch's theory. Song measured the SHG from thin films of rubidium deposited onto a cold (100 K) Ag(110) surface. In addition to the large enhancement of the SH at monolayer coverage relative to the bare silver substrate, which had been noted by others, Song observed strong oscillations of the SH signal as a function of film thickness for films in the 10-100 Å range. These oscillations were identified with Friedel density oscillations in the rubidium, as predicted by Liebsch's theory. The theory does not yet give a complete quantitative description of the rubidium-silver interface or the observed dependence of amplitude on laser wavelength, but results thus far are encouraging.

The epitaxial CaF<sub>2</sub>: Si(111) interface was the object of an experiment described by T. Heinz, IBM, Yorktown Heights. The interesting feature was a strong resonance in the wavelength dependence of SH intensity at the effective interface band gap for this system, 2.41 eV. Ph. Avouris commented that the scanning tunneling microscope sees a gap of just this magnitude, which is independent of CaF<sub>2</sub> coverage from one monolayer to about 30 Å.

Highlighting the versatility of SHG, G. Richmond, University of Oregon, described research on thin metallic films grown electrochemically on noble metal electrodes and measured in situ. Changes in the SH signal could be observed as one or two monolayers of metals such as thallium were deposited or desorbed.

To end this incomplete survey of the surface SHG sessions, it is appropriate to mention a paper by H. Tom, AT&T Bell Laboratories, Holmdel, on femtosecond SHG in single-crystal Si(111) and Si(100), which revives an old controversy about laser annealing. The experiment measured an anisotropic part of the nonlinear sus-

ceptibility, a tensor quantity that could be correlated with bulk crystal structure. When surface was excited by a 75-fs pulse of sufficient intensity to melt the silicon, the order-dependent component of the SH signal disappeared in less than 150 fs, but an isotropic component that could be associated with the metallic melt phase decayed in 300 fs. Since significant atom displacements cannot occur in 150 fs, this component was attributed to electronic rather than atomic disorder. Those who remember the laser annealing debates of the early 1980s may recall J. Van Vechten's strong advocacy of an electronically disordered, premelt state in silicon, which had faded from conference programs and journal pages for lack of clear experimental support. Although not proclaimed as a proof, Tom's data certainly suggest reconsideration of the concept. The potential range of applicability of the phenomenon is, at most, considerably narrower than originally envisioned, since conventional lattice melting has now been established experimentally as the source of laser annealing under a wide variety of circumstances.

## Summary

As this survey suggests, a lot of surface science was touched on in these 5 days. Without the guidance of previous conferences, the organizers were able to achieve a well-focused program with sufficient variety and quality to be interesting throughout. It was evident that there are many ways in which lasers can provide important data not otherwise accessible and that this approach is yielding some of the most exciting developments in experimental surface science. The conference did exactly what its organizers intended: it created a new perspective on surface science.

# MATHEMATICS

## Scientific Research Programs at the University of Rome and University of Naples

by Richard Franke, formerly the Liaison Scientist for Mathematics and Scientific Computing in Europe and the Middle East for the Office of Naval Research European Office. In September 1989, Dr. Franke returned to the Naval Postgraduate School, Monterey, California, where he is a Professor of Mathematics.

### University of Rome

My visit to the Universita di Roma "La Sapienza" was arranged through Professor Francesco Zirilli. The university has about 150,000 students; the enrollment in

mathematics is about 500 per year. The Department of Mathematics is at Piazza Aldo Moro on the grounds of the old university. The Department of Mechanics and Aeronautics is located in another building some 3 km. away, not far from the Coliseum and adjacent to San Pie-

tro in Vincoli. A third part of the school, which I did not visit, is located elsewhere in Rome.

**Department of Mathematics.** The U.S. Air Force Office of Scientific Research Office has supported Zirilli for several years. He previously worked on optimization problems from the point of view of finding their solution as a stable equilibrium point of a system of ordinary differential equations. Some properties of the problems may then be derived from the differential system, with the system then being solved using numerical techniques. Other methods may be cast into a special instance of this scheme, and the point of view afforded may allow faster convergence by having a better idea of how to choose parameters (such as a stepsize) for which there is now a better interpretation.

Zirilli's present work is toward solution of the inverse acoustical scattering problem. The direct scattering problem is to solve the Helmholtz equation in 3-space outside of a given body  $D$  containing the origin, subject to given conditions on the boundary of the body and a far field condition (the Sommerfeld radiation condition) on the scattered wave, with given input plane waves. The inverse problem is to find the boundary of the body, given the input wave, some measurements of the total wave (from which the scattered wave can be inferred), again subject to the boundary and far field conditions. Zirilli's work has assumed an acoustically soft body (Dirichlet boundary condition), although other conditions can be used and are necessary, depending on the type of object from which the waves are scattered. It is also assumed the body is smooth.

Zirilli and his group's work is based on and extends the work of Colton and Monk. In a practical problem, the input wave is from a few directions, and the measurements of the total wave can be performed in only a few directions. The ideas of the algorithm can be summarized in four steps.

1. It can be shown that the scattered wave can be expressed as a function which has the form  $\exp(ikr)/r F(x, k, \alpha) + O(r^{-2})$ , where  $x$  is a unit vector toward position  $x$ ,  $k$  is the wave number, and  $\alpha$  is a unit vector in the direction at which the far field scattered wave is observed. Approximate values of  $F$  are obtained by measurement at discrete points. The (discrete) Fourier transform (in terms of spherical harmonics) of  $F$  is computed. The system of equations for the Fourier coefficients is ill-conditioned, and a "parabolic regularization" method is used, obtaining the solution of the system of nodes by numerical integration using an L-stable method.

Use of symmetry can decrease the number of unknowns. The number of coefficients that can be computed depends on the number of known data.

2. From the far field patterns, the Herglotz kernel,  $g(x)$ , is computed. The Herglotz kernel is defined by an inte-

gral equation over the boundary of the body,  $D$ .  $g$  is solved for by finding its Fourier expansion, using the integral equation, orthogonality properties, and symmetry where applicable.

3. The Herglotz wave function is computed as the Fourier transform of the Herglotz kernel. The integrals here can be evaluated in terms of spherical Bessel functions and their derivatives, which are elementary functions. It is convenient to use polar variables from this point.

4. It is assumed that the boundary of the body  $D$  contains the origin in its interior, is starlike with respect to the origin, and has bounded radial coordinate  $r = f(\emptyset, \Theta)$ . If  $D$  is a Herglotz domain, then  $f$  and the Herglotz wave function satisfy a functional relationship. This relationship implicitly defines  $f$ , although the relation also includes other sets. The value of  $f$  at the pole can be found by solving a single nonlinear equation. To find  $f$  for a fixed  $\Theta$ , this value is then used as an initial value in the initial value problem obtained by differentiation of the implicit relation. A similar strategy is used in the variable  $\emptyset$ . Numerical solutions of these equations are obtained by Runge-Kutta methods, and can be carried out in parallel. Only solutions that generate closed surfaces are proper solutions. Zirilli and his coworkers give some examples of reconstruction of objects. They first solve the direct problem for a given body to find input conditions for the inverse problem. The body is then reconstructed using the method outlined above (see Aluffi-Pentini, et al.). The examples show the method works quite well for exact data and smooth bodies, with performance deteriorating for noisy measurements and nonsmooth bodies.

Zirilli and his students are considering the problem of acoustical scattering from bodies with edges. Initially, they are considering the case where the body is regular (in particular the platonic solids), investigating uniqueness properties and whether it can be easily determined which of the solids the body is.

I also talked with Professor Stefano Levialdi about his work in three areas.

1. Levialdi is involved in the beginning of a Computer Science curriculum at the University of Rome. This course is envisioned as being quite high in its content of mathematics and physics in the first years of study, with considerable emphasis on the theoretical aspects of Computer Science topics. For example, consider computer languages. It is felt that specific languages should not be formally taught, but that with a suitable background in languages, the student will be able to make intelligent tradeoffs between languages for a particular application, and then be able to self-learn the formal part of programming in that language.

2. Levialdi is interested in multiprocessor applications to image processing. A recent review of computer architec-

tures for image processing purposes, especially parallel architectures, is given in Cantoni and Levialdi. Levialdi has been very active in organizing and participating in conferences and has coedited several proceedings.

3. Regarding visual languages, Levialdi feels that most unskilled persons relate more easily to highly technical matters when presented a visual image. A simple example is using icons for selection of tasks to be carried out by a computer. A slight extension to the idea is using icons to enable a nontechnical word processor operator to enter complicated equations simply by selecting stencils which are then filled in with the proper symbols. This assumes that the equation is written so that it can be "read" by the operator; of course, the system can be used by a technically oriented person as well. One advantage of such a system is that it is "what you see is what you get" (WYSIWYG), so that the equation appears on the screen as it will on paper, unlike text processors; e.g., TEX. However, a potentially much bigger area of application is to expert systems for diagnosis and repair of technically complicated systems, such as electronic and mechanical systems which are used in radars, telephones, airplanes, and automobiles. Such a system, with a specific example in radar repair, is given in Cinque, et al. Levialdi is the program chairman for the 1989 IEEE Workshop on Visual Languages to be held in Rome in October 1989.

**Department of Mechanics and Aeronautics.** I visited with Professors Renzo Piva and Luigi Morino at the Department of Mechanics and Aeronautics. They explained that the interests of the department were in several areas, especially in fluid dynamics and the associated numerical analysis, and some work in mechanical vibrations and acoustics. Some experimental work is also performed within the department and the results are used as test cases to verify their computer codes. I will discuss briefly some of the activities of the department.

Some recent work on two-dimensional hypersonic flow is described in Valorani, et al. The work is relevant to the HERMES shuttle, and considers the finite rate chemical processes in a hypersonic flow field. The main problems occur with the stiffness of the equations at near-equilibrium conditions, and the large gradients of concentrations. This paper proposes a shock fitting technique and variable step integration along the streamlines for the energy and species conservation equations. An implicit scheme is used for the species equations. Future work is toward more complicated reacting flows with embedded shock waves and toward increasing the efficiency of the method.

The use of a vector Green's function method for unsteady Navier-Stokes equations is developed in Piva and Morino. While the solution of the compressible unsteady Navier-Stokes equation is given in closed form, they suggest some approximations that are easier to handle. The

end goal of the development is the use of the resulting integral formulation in a boundary element method for the approximate solution of the equations, although that is not carried out in this particular paper. Further work on boundary element methods for fluid dynamics is described in Piva, et al. Morino and coauthors have contributed some chapters to a forthcoming book on boundary element methods, one of which is cited below. It contains the development and a review of the literature in the use of boundary element methods for the analysis of potential aerodynamic flows around aircraft. Applications to airplanes, helicopters, and propellers is a particular emphasis.

## University of Naples

The Universita' di Napoli is spread out around Naples with a total student population of about 100,000 with about 12,000 students in the engineering school. I visited at the university through the courtesy of Professor Carlo Savy of the Dipartimento di Informatica e Sistemistica, and spoke with Savy and a graduate student, Ing. Giorgio Ventre. They are involved in several projects related to parallel and supercomputing, some of which I will discuss in more detail. Savy is the director of a new initiative of the Consiglio Nazionale della Ricerca (CNR) and the Universita' di Napoli which is called the Centro di ricerca sul Calcolo Parallelo ed il Supercalcolo (CPS). I will first discuss some of the facilities and recent work of the department and then the plans for CPS.

**Department of Computer Science and Systems.** The computational facilities of the department are extensive, consisting of more than 100 PC- and PC/AT-type machines plus some Sun workstations, all of which will eventually be networked. A Sun is the host to a Transputer board with four processors. The department has ordered a Meiko M10 parallel machine with 16 processors. Each of the 20 departments at the school has a Unisys 5000, or a comparable NCR Tower machine, all of which run UNIX. In addition, they have access to the main computer at the Interfaculty Center for Computing Service (CISED), a Univac 1100/91. In turn, this computer is connected to other consortia of university computer centers, giving access to machines such as the CRAY XMP/48 at CINECA, near Bologna. Other machines are available in Naples, particularly, an Inmos machine with 64 T800 transputers which belongs to the CNR. The CNR has ordered a 256 processor Meiko computing surface. Planned equipment acquisitions for the CPS will be mentioned later. One problem for southern Italian universities relative to those in northern Italy is that the principal industrial organizations, including their research facilities, are in the north. Thus, few funds for research and hardware have been available for the southern universities. Some alleviation of this problem for the University

of Naples is anticipated with the establishment of the Italian Center for Aerospace Research (CIRA), with whom close interaction is expected. The CIRA is being established by a consortium of companies, and eventually 600 researchers will work at the center in nearby Capua.

Ventre explained to me one of the important areas of work in the department. He is working on a language for parallel processing called Distributed C (DISC) which is designed for systems that have several autonomous processing units with local memory and that are connected by a communication network. The language is a superset of the C language, and the first pass of the compiler converts DISC to conventional C. Obviously, this allows the direct incorporation of sequential C programs into DISC. The two guiding principles behind the language are the direct management of parallelism, and modular programming. The initial multiprocessor host machine is the transputer-based board for the Sun workstation. The communicating sequential processes (CSP) computational model of C.A.R. Hoare is being followed. At the present, the DISC language and the DISC run-time support system have been defined, with work proceeding on the DISC development environment. An important practical aspect of the language is that individual modules are compiled individually and later linked. Ventre has written a DISC compiler and a linker for the modules. Now only a preliminary version of the run-time monitoring and debugging aids are available with further refinement being carried out. This work will be carried forward under the new CPS. An early version, a recent description, and the language definition are given in the three references, Iannello, et al. The point of view is that the actual hardware must be transparent to the programmer, and that the high level language deals with virtual multiprocessors. The actual architecture of the host machine is to be dealt with at a low level and normally not be part of the applications programmer's worries. This allows a reasonable degree of portability since machine dependencies are isolated into a few modules with well defined interfaces.

Additional work in the department is related to synthetic aperture radar, in conjunction with the Department of Electronic Engineering, supported by the Italian Space Agency (ASI) and a company--Selenia. This work is related to earthquake prediction through monitoring of ground movements. Since Naples is subject to earthquakes, this is an especially appropriate study.

Other members of the department are involved in process control. This work partially supports Ansaldo, a research center that focuses on transportation systems.

The image processing group participates in another very interesting project that relates to electronic restoration of artwork found at sites in Italy, such as Pompeii. This project is the work of a consortium of companies in cooperation with archaeological experts under the name

NEAPOLIS, which I was informed is Greek for Naples. In this project, damaged wall paintings are digitized and displayed on a high-resolution color monitor. Using colors from other parts of the picture, or possibly combinations of them, the artistic restorer electronically repairs damaged areas of the picture. Unlike restorations to such paintings as *The Last Supper* of Leonardo di Vinci at the Church of Santa Maria delle Grazie in Milan, the original pictures are not restored. Along with information about the ruins, the restorations can be made available to tourists. A similar endeavor involved the electronic reconstruction of partially destroyed buildings by comparing remaining ruins with other similar, but less damaged ones. Another project was using image processing to allow reading of damaged papyri.

**Parallel Computing and Supercomputing Research Center.** The CPS is funded by the CNR to establish a parallel computation research center in southern Italy. An initial allocation of about 15 billion lire (about \$11 million) for equipment was made. About 1 billion lire per year will be used to support about 10 researchers plus 4 technical support persons. The center will be established in an office building within 1 km. of the location of the Department of Computer Science and Systems. The goals of the center strike a balance between research and service to universities and companies in southern Italy, to include research in the field of parallel systems; training activities for universities, research centers, and companies; and supercomputing services.

There will be close cooperation with other departments at the University of Naples and other CNR institutes. Research cooperation is to be carried out between CPS and the following:

- Department of Applied Mathematics
- Department of Computer Science and Systems
- Institute for Parallel Computing (IRSI), a CNR institute in Naples
- Institute for Applied Mathematics (IAM), a CNR institute in Naples
- Institute of Cybernetics, a CNR institute in Naples
- Others, including CIRA.

Each of the cooperating facilities will be networked to the center through workstations. They will use UNIX as the uniform operating system on the network. Close cooperation with those interested in applications is considered to be a very important aspect of the plan.

The primary effort will be in parallel systems, with the supercomputing activity principally a service using a mini-supercomputer such as a Convex or Alliant, with access to the Cray at CINECA. New applications and software development for supercomputers will be achieved with the Department of Applied Mathematics and other applications-oriented partners.

The planned acquisition of massively parallel computers is anticipated to be those based on the transputer, such as the Meiko computing surface, and perhaps a system with hypercube architecture. A priority list for machine acquisition is being developed.

## Final Comments

The work being achieved at the University of Rome in applied mathematics is interesting and potentially very useful since fluid flow about aircraft structures and acoustics is important. Work on visual communication with computers is becoming more important and refinements are necessary. The parallel processing project at the University of Naples is ambitious and complements efforts of another CNR project (ESNIB 89-08:27-34). Since the need is great, languages for parallel processing are being investigated at numerous places. Whether a small group such as that at Naples can define and implement a viable candidate will be interesting to follow.

## Bibliography

Aluffi-Pentini, F., E. Caglioti, L. Misci, and F. Zirilli, "A Numerical Method for the Three Dimensional Inverse Acoustic Scattering Problem with Incomplete Data," ITMAS Workshop on Numerical Analysis, Merida, Mexico, January 1989.

Aluffi-Pentini, F., E. Caglioti, L. Misci, and F. Zirilli, "A Parallel Algorithm for a Three Dimensional Inverse Acoustic Scattering Problem," to appear in the *Proceedings of the International Meeting on Parallel Computing*, Verona, Italy (1988).

Cantoni, V. and S. Levialdi, "Multiprocessor Computing for Images," Proceedings of the IEEE 76(1988), 959-969.

Cinque, L., M. Crispoldi, F. Fontana, and S. Levialdi, *A Multi-Level Expert System for Repair Applications*, manuscript.

Colton, D., and P. Monk, "The Numerical Solution of the Three Dimensional Inverse Scattering Problem for Time Harmonic Waves," *SIAM Journal on Scientific and Statistical Computing* 8,(1987), 278-291.

Iannello, G., A. Mazzeo, C. Savy, and G. Ventre, "A System for Parallel Software Development," pp. 304-307, *Proceedings of the 12th IMACS World Congress*, 1988.

Iannello, G., A. Mazzeo, C. Savy, and G. Ventre, "Parallel Software Development in the DISC Programming Environment," to appear in *Future Generation Computer Systems*.

Iannello, G., A. Mazzeo, and G. Ventre, "Definition of the DISC Concurrent Language," submitted to *ACM SIGPLAN Notices*.

Morino, L., and K. Tseng, "A General Theory of Unsteady Compressible Potential Flows with Application to Airplanes and Rotors," to appear in *Developments in Boundary Element Methods, Vol 6: Nonlinear Problems of Fluid Dynamics*, P.K. Banerjee and L. Morino, eds., Elsevier Applied Science Publishers, Barking, UK, 1989.

Piva, R., and Luigi Morino, "Vector Green's Function Method for Unsteady Navier-Stokes Equations," *Mecanica* 22 (1987), 76-85.

Piva, R., G. Graziani, and L. Morino, "Boundary Integral Equation Method for Unsteady Viscous and Inviscid Flows," in *Advanced Boundary Element Methods*, Th. A. Cruse, ed., Springer-Verlag, 1988.

Valorani, M., M. Onofri, and B. Favini, "On the Solution of Nonequilibrium Hypersonic Inviscid Steady Flows," *27th Aerospace Sciences Meeting*, Reno, NV, January 9-12, 1989.

# Third International Conference on Supercomputing

by Richard Franke

## Introduction

This conference, originally planned to be held in the U.S., was held in Heraklion, Crete, on June 5-9, 1989, under the sponsorship of the Computer Technology Institute in Patras. The previous two conferences were held in Athens, Greece, and St. Malo, France, respectively. The conference attracted about 140 attendees from all

around the world. There were eight invited presentations, about 50 one-half hour presentations, which appear in the proceedings, and about a dozen 15-minute presentations. The papers covered a wide variety of issues concerning conventional vector supercomputers as well as massively parallel systems, including topics such as algorithms and applications, compiler techniques and analysis, languages for parallel processing, performance of

various components of systems, and new Japanese computer systems. Since most of the papers appear in the Proceedings, I will concentrate my discussion on the invited talks and the panel session on languages and compilers.

## Invited Talks

The first talk was nontechnical, "ESPRIT and its Practical Results," by Dr. Jean-François Omnes of the European Economic Community (EEC) Information Technologies--European Strategic Program for Research and Development Information Technologies (ESPRIT) organization. Omnes reviewed the work of the project to aid European information technology (IT) companies to restructure for the post-1992 situation. Basically, the project's focus is to promote cooperation between European companies, provide them with basic technologies for the 1990s, and pave the way for industry standards. The first phase of the project involving an expenditure of some 1.5B ECUs (an ECU is currently about \$1.08) has been completed successfully. One of the projects was the Supernode project resulting in the T800 Transputer that is being used in a number of multi-processor applications, and looks quite promising. The ESPRIT II program is now under way, funded at a level of 3.2B ECUs. The projects being supported are in microelectronics, information processing systems, and IT application technologies, along with a small amount of basic research funding. There is stress placed on cooperative projects between companies and universities and across country borders. Emphasis is on Supernode II and high performance, low cost, parallel systems. Omnes noted that the European market share is increasing, along with investment by the IT companies. Investment is increasing faster in Europe than in either the U.S. or Japan. How much these increases are because of ESPRIT is somewhat speculative, but there is no doubt it is important.

Dr. Robert Haber, National Center for Supercomputer Applications, Champaign, Illinois, spoke on "Interactive Visualization in Scientific Computing." Haber outlined the usual steps in the process from scientific computations to visualization: simulation -> data enrichment/enhancement -> derived data -> visualization mapping -> rendering -> displayable image. The process generally proceeds from hard to easy (at least, less hard). Haber showed by video examples that it was sometimes (I would say: usually) necessary to use interactive techniques to obtain suitable displayed images from the derived data. One example was the propagation of a crack in a plate, where a colored surface was displayed above the plate, the height of the surface representing the kinetic energy density, and the color representing the

strain energy. Without the appropriate color mapping, little information about the strain energy radiating from the crack tip was shown, while an interactive change in this mapping revealed waves of energy propagating from the crack tip. Haber noted that three-dimensional simulations yield information, which is much more difficult to process for visualization. Examples noted were such things as tensor fields (e.g., how does one show the Lamé stress ellipsoid?), turbulence (two-dimensional cross-sections are surely not the answer), and thunderstorms (contours of vorticity, where vorticity level varies with time shows some interesting things). With supercomputers now widely available and the emergence of high performance graphics workstations at reasonable prices, communication of the often vast amount of information is still a big problem. Although it is considerably relieved from when a magnetic tape carried across the campus by hand was the best way to do it. Haber closed by listing some trends and directions for the future: new visual abstractions, direct volumetric rendering, increased interactivity for exploration, distributed simulation/visualization systems, and menu-driven high-level tool development.

Dr. Vivek Sarkar, IBM Watson Research Center, Yorktown Heights, spoke on "Delivering Supercomputer Performance to the User." Sarkar discussed IBM's PTRAN program for translating serial Fortran code into IBM Parallel Fortran. The goal is to detect and manage parallelism, while paying some attention to execution time analysis in critical areas of the program. Two types of dependencies must be analyzed--data dependencies and control dependencies. In the first instance, loop transformations may be made once the data dependencies have been analyzed. Certain control conditions may imply that parallel execution may be permitted, but data dependency must still be investigated. The initial approach in PTRAN is to use control sequencing to satisfy data dependencies, which simplifies the problem, but may not enable exploitation of all parallelism. Run-time behavior is estimated from loop frequencies, branch probabilities, and average execution times, which depend on the characteristics of the target machine. For the future, Sarkar expects they will investigate the fact that there may be a lot of large "dusty deck" codes for translation to run on the IBM 3090 parallel processors. Further, he expects they will want to allow explicit parallel constructs in the input program.

One of the most interesting talks, and one that proposed a start on the solution of a very difficult problem, was given by Professor John Gurd, University of Manchester, U.K. entitled "Comparing the Performance of Different Styles of Supercomputers." Gurd noted that there are very different approaches to obtaining supercomputer performance, and that all have some very difficult hurdles to overcome. It is not easy to compare

development costs and performance benefits of the various approaches; and historically, such evaluations have been poor. Gurd outlined the history of computer evolution. Generally, the evolution is driven by the applications, from a high level mathematical specification of the problem in continuous terms, to the algorithmic discrete level, to the programming level which implements the algorithm, to the realization as a program executed on hardware. According to Gurd, computational paradigms are hardware-driven and decisions on which hardware to purchase are often based on arbitrary reasons. This fixes the methodology and tools that can be brought to bear on a particular problem, and also limits the choice of languages.

Thus, the complete top/down approach that should drive the problem-solving process cannot be carried out. The costs in various steps are not well understood, nor are the costs of switching to another computer along the way. This is particularly true in the case of a large investment in existing programs in a given language, where the one-time cost of converting completely overshadows the fact that decreases in overall development costs in future projects would make it profitable to switch.

Gurd suggests that a large project should be undertaken to attempt to quantify the costs and benefits of various approaches in a way that would make comparisons possible. He and his coworkers have begun such a project, and preliminary results are available (see Gurd, et al.). He welcomes any help from those who share his belief that this kind of investigation is needed. The units of cost may be time, money, or skills. There are many kinds of costs; e.g., development costs; marginal costs (the usual one, since most projects build upon much previous work); incremental costs (caused by changing the status quo); and opportunity costs (including features that are "too good to miss" but whose real cost comes later). Balanced against these are performance benefits during execution of the program.

The experimental framework in which Gurd is working contains the following features:

- Solve problems in many different ways (he notes this is probably boring for end users, but must be done by someone)
- Use a set of sensible and representative problems
- Agree on methods and measurements (necessary)
- Keep accurate and open records (vital)
- Work bottom/up in filling in the details of the mapping space.

For each problem, a base case should be available that would be very cheap to develop but expensive to execute, but which then serves as an upper bound.

The initial experiment has been carried out as follows:

- Set of general problems and control problems was defined (spanning the range from embarrassingly parallel to very serial)
- Set of algorithms for the problems was defined
- Algorithms were implemented in many languages and different styles
- Programs were compiled and run on parallel systems and some "control" uniprocessors.

The execution time in elapsed cycles (a cycle is taken as the time to get one result), and some other things, were measured. Gurd noted that while some of these things have been done in the past, a large problem is that there is not much uniformity since most investigations have been for specific problems or specific processors, and what was interesting to measure depended on the particular situation. For the future, Gurd wants to complete the early investigation, extend it to other machines, and assess development costs as well as document the performance record.

In a somewhat similar vein, Dr. Paul Messina, Director of the Concurrent Supercomputing Facilities, CalTech, spoke of his work on "Performance Measurement of Advanced Architecture Computers." Messina described his work as being somewhat in the spirit of Consumers Report. The reason for this approach is because of the rapid developments in parallel computer architecture and introduction of parallel machines, and the nearly-as-rapid disappearance of some manufacturers. To be useful to the user community with reference to particular brands, quick response is necessary, although certainly the viability of some architectural approaches may transcend the financial vagaries of the marketplace. What has been done is to create a catalog of applications programs, originally implemented on various vector supercomputers and parallel computers, along with a few that were written for specific machines to which they have ready access. These programs are typically written in Fortran or C language, some are portable, some are scalable, or have other nice properties. The programs are from high-energy physics, signal processing, chemistry, fluid dynamics, plasma physics, and (of course) some linear algebra codes. The first attempt was to use these codes on other machines much as a user might; get them running with a minimum of effort, then spend some time (up to 40 hours) to fine tune them for the particular machine. At this point, it was also desirable to enlist the aid of experts from the applications area (the originator of the program, if possible) in order to make sure the process was up to date, that the problem sizes were appropriate, and that other such details were correct. The typical program was a research program of some 1,000 to 4,000 lines of code. In this context, some of the codes had been used on massively parallel machines to obtain new research results. The programs were run on a variety of machines (this is

not a complete list)--vector supercomputers such as the Cray XMP, Cray 2, ETA-10, and Cyber 205; minisupercomputers such as the SDS-40; shared memory multiprocessors such as the Alliant FX/8; and a variety of parallel machines such as hypercubes (NCUBE and Intel), Sequent Balance, and Meiko computing surface. The multiprocessor machines were all run using one or a few processors to the complete set. The amount of data to be assimilated and then trying to make sense of the results is somewhat staggering. By plotting execution time (or MFLOPS rate) for each machine versus number of processors to obtain a performance graph, some interesting things emerge.

Some observations are: some problems are too small to make use of all nodes of the 512 node NCUBE, while scaling up the problem makes very good use of them; some problems are inherently not vectorizable and vector supercomputers perform at a fraction (less than 1 percent) of their peak rates; some problems do not run faster with several processors of a shared memory machine than they do on one processor; some applications should not be written in certain languages for certain machines.

Some of the conclusions reached by Messina are: (1) 1989 is the year of the parallel (meaning more than 64 processors) supercomputer, with some new results being obtained on these machines at computational rates similar to vector supercomputers; (2) shared memory multiprocessors are easier to program than local memory machines; (3) massively parallel machines will probably make the best inroads against vector supercomputers for problems which do not vectorize; (4) and with recent and anticipated developments, vector supercomputers will maintain their supremacy in GFLOP rates and remain in use for problems that do vectorize well.

Dr. Raul Mendez, Institute for Supercomputing Research, Tokyo, discussed the Japanese challenge in the supercomputer area in "Japanese Supercomputers: The Second Wave." According to Mendez, there is an installed base of 125 supercomputers in Japan, predominantly Fujitsu VP series, but also including 17 Cray machines, and one ETA (rip). Only 39 percent of the machines are in government and universities, with the remainder in industry. The predominant use of the Cray machines is in the automobile industry and they are used because the principal auto crash simulation program (from a third party vendor) has not been ported to the Japanese supercomputers.

Fujitsu announced the FACOM VP2000 series and NEC the SX-3 series recently. This was followed by Hitachi's announcement of its S-820/80 machine. The S-820/80 computer has a peak computation rate of 2.2 GFLOPS per processor with up to four processors available, and up to 512 Mbytes of memory. The technology is BiCMOS, allowing the machine to be air cooled. Clock time is 4 ns for the vector processors, and 8 ns for the scalar

processors. The NEC SX-3 machine has a 2.9-ns clock and 2 GBytes of memory. Each processor can have up to 16 vector pipelines capable of producing one result per clock time, for a peak computational rate of 5.5 GFLOPS per processor; up to four processors are available. The Fujitsu VP 2000 machine has similar capabilities. The latter two machines are outgrowth of a Ministry of Trade and Industry project to develop high speed computers, while the Hitachi machine is an independent development.

Mendez also discussed his work in benchmarking various supercomputers over the past several years. The S-820 is some 2 to 5 times faster than any previous machine tested in simple application (primarily various fluid dynamics codes) programs which vectorize well, but less impressive in scalar mode. Mendez noted that performance on certain computational kernels is not sufficient to judge overall performance. In compiler technology, simply looking at the number of loops vectorized is not enough, this being poorly correlated with execution time; and in his experience, Fortran compilers for Japanese machines have sometimes crashed on very large programs.

Mendez mentioned several problems and deficiencies that confront the Japanese. Connectivity is very poor, with most supercomputers being stand alone systems. Support software such as postprocessing for visualization is underdeveloped. High-speed communication lines are very expensive so most links between computers are low speed only. The physical facilities for computer sites also tend to be poor, with not enough space, and power supply problems are common. As mentioned above, third party software availability is poor.

Presently, there is very little work on parallel supercomputers in Japan, with some low level funding at the university level. Thus, the three Japanese manufacturers are all producing machines with a design approach similar to Cray (a few very high speed vector processors, shared memory) for essentially the Japanese market since the installed base of Japanese supercomputers outside of Japan is small. Further, there are no minisupercomputer manufacturers as in the U.S. In the present situation, Mendez feels that Cray faces more competition from U.S. manufacturers than those in Japan.

The final session of the conference was a panel discussion on compilers and languages. Panel members were Mark Furtney (Cray Research), Dennis Gannon (University of Indiana), John Gurd, (Manchester University), Yoichi Muraoka (Wasada, Japan), Rishiyur Nikhil (MIT), Alex Nikolau (University of California, Irvine), Vivek Sarkar (IBM Watson Research Laboratory), William Wolfe (Oregon Graduate Center), and Constantine Polychronopoulos (Center for Supercomputing Research and Development, University of Illinois). Some of the points made during the initial statements, and the following question and answer period were

- Furtney - Cray is successful because they have a fast, general purpose machine, with good software and compilers. The software is crucial, and their new automatic multitasking software (Autotasking, tm) is working very well.
- Gannon - Compilers need to be improved; inner loops are handled well with current compilers, but outer loops less well. Big outer loops almost always need some reorganization to parallelize. Languages need to be developed to help handle such problems, with neither Fortran nor C seeming to be right. Gannon is working on an interactive Fortran/C analyzer called Faust that will let the programmer help decide whether loops can actually be parallelized or not, or to tell the programmer why a loop cannot be parallelized.
- Gurd - Hardware parallelism will increase, to a few hundred or a thousand processors, but probably not more. Machines should be widely available, and the present user community should be communicating pitfalls to potential users. He feels compilers should disguise parallel hardware, but wonders whether existing programs can be reasonably unraveled by compilers. Languages for parallel machines should be closer to the problem description, with parallelism being implicit rather than explicit. At present, it is difficult to change a program from one parallel machine to another. Standards must be developed.
- Muraoka - The user is king, and doubtful if parallel data and parallel control systems can be completely successful because the user must be an expert. In his opinion, message passing systems cannot get enough parallelism. Language and hardware need to be separated, and a unified approach to theory and implementation is necessary.
- Nikhil - Functional programming languages must be developed for parallel applications, noting that most programs are deterministic. The distinction between numerical and symbolic processing will disappear since the need for symbolic processing for visualization, input, choosing numerical methods, and focusing on particular aspects are very important. Fortran is inadequate and Lisp-like languages are needed. Programs generally over-specify ordering, from which the compiler then tries to determine parallelism. Functional languages where each location receives a stored value once have a better chance for overlap of computation, but require much storage. Nikhil feels this may not be enough, but that functional languages are getting better.
- Nikolau - In favor of (very) fine grain parallelism since it makes available nearly all parallelism possible. This should be exploited as possible at compile time with a global analysis, which results in low run-time overhead. Nikolau thinks very long instruction word machines and long pipeline processors, rather than vector processors, are the key.
- Sarkar - Sees a need for a general virtual parallel machine that would include many realizations at the hardware level. There is a need for various languages--serial, parallel, and functional--that would be compiled onto the virtual machine and then ported to the actual hardware. The serial language would be automatically parallelized. The parallel language would contain explicit parallelism, while the functional language would contain implicit parallelism.
- Wolfe - Initial comment was that no code is better than slow code. His view is that compilers should train the user in how to write code for it. As an example, he cited early vector Fortran compilers that would indicate when loops could not be vectorized, so the user could then remove or modify the offending portion of the code. In the interim, of course, the compilers have become much "smarter."
- Polychronopoulos - Run-time overhead is the main problem, not Amdahl's law. He thinks the language should extract the minimal parallelism since then the code can run on all machines, assuming the appropriate compiler is available. The operating systems should be adaptive, decide whether batch or multiuser mode is best, and decide whether or not parallel execution is appropriate. The hardware should be able to handle scheduling/synchronization and process creation management.

During the question and answer period, many of the above ideas were amplified. I believe two of the important ideas expressed were that cost-effective computation is more important than speed, and that the hardware is really the cheapest part of the process. There are exceptions to that rule, such as in computational fluid dynamics and computational physics, where raw speed is very important. Reservations were expressed concerning the recently adopted Fortran 88 standard, as well as the new C standard, with the C standard apparently having very serious deficiencies for numerical calculations.

## Final Comments

This meeting was a truly international meeting, with significant numbers of speakers and attendees from the U.S., Europe, and Japan. The contributed talks are contained in the Proceedings distributed at the meeting and thus were several months old. On the other hand, unlike meetings where the papers are due after the meeting, they were immediately available for study before the talk was

given. The invited talks tended to embody the most recent information available, and I hope I have managed to convey here the most interesting parts of them and the panel discussion on current issues in languages and compilers. The fourth ICS meeting will be held in Amsterdam on June 11-15, 1990.

## References

Proceedings, 3rd International Conference on Supercomputing, Heraklion, Crete, 5-9 June 1989, Association for Computing Machinery, New York.

Gurd, J.R., A.P.W. Böhm, and D.F. Snelling, "Comparing the Performance of Different Styles of Supercomputer," preprint.

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# Surfaces in Computer-Aided Geometric Design

by Richard Franke

## Introduction

The Mathematisches Forschungsinstitut Oberwolfach is a conference facility located in the Black Forest village of Oberwolfach-Walke, Federal Republic of Germany. The facility is used almost exclusively for hosting small mathematical workshops and meetings, with at least one meeting being held each of 50 weeks per year. The facility is funded in part by the Volkswagen Foundation, allowing modest charges to be made for living expenses during the meetings. The complex is self-contained with dormitory space and family style dining facilities greatly enhancing contact between participants. In some cases attendees must be housed at hotels in the village, although more dormitory space is presently being added. In addition, the institute can provide space for individuals who wish to visit and use the excellent mathematical library, including access to remote databases. Word processing and other personal computing services are available on Macintosh II computers.

The Surfaces in Computer-Aided Geometric Design (CAGD) meeting was the fourth in a series of workshop/conferences held at Oberwolfach; the first was held in 1982. The conference was organized by Professors Robert E. Barnhill (Arizona State University), Josef Hoschek (Technical University Darmstadt), and Wolfgang Böhm (University of Braunschweig). The total attendance was about 60, of which about 40 gave presentations of recent research results. The attendees were primarily from European countries and the U.S., with a few from countries such as Israel and China. I will describe in some detail a portion of the presentations, and give short descriptions or abstracts for the rest. The proceedings of the meeting will appear in *Computer-Aided Geometric Design*, and also as a separate book (see Barnhill).

## Geometry Processing and Surfaces on Surfaces, Robert E. Barnhill, Arizona State University

Geometry processing is the extraction of geometric features from a given surface or surfaces. Examples include surface-surface intersections, reflection lines, and curvature plots. Curvatures depend on second derivatives, and thus yield more information about the quality of the surface than reflection lines, which depend on first derivatives. Surfaces defined on surfaces are important for a variety of problems, the most apparent being functions defined on the surface of the earth. Other examples are pressures on the surface of a wing and temperatures on the outer surface of a spacecraft. Some methods of defining such interpolation functions were mentioned, especially convex combinations by distance weighing, distance being measured along the geodesic.

## Surface Operations in Higher Dimensions, Christoph Hoffman, Purdue University

Hoffman noted that certain operations on surfaces may be more easily carried out by embedding the process into higher dimensional space. For example, the description of surface offsets can be described by a system of four equations in four unknowns. An extension to this is the Voronoi surface, the surface equidistant from two given surfaces. The latter idea gives an easy way of constructing variable radius "rolling ball" fillets between two surfaces. Depending on the way the surfaces are described (implicit or parametric, or one each), the result is a system of up to eight equations in ten unknowns. The simplification of such systems of (polynomial) equations was discussed through the use of Gröbner bases, for which reasonable software is becoming available. The process should be considered as an alternative to implicitization which results in more equations, but lower degree.

## Scattered Data Interpolation Based Upon Minimum Norm Networks, Helmut Pottmann, University of Vienna

A number of interpolation and approximation schemes for scattered data are based upon minimizing some pseudonorm of the approximating function. One example is the minimization of a pseudonorm of a network of curves over the edges in a triangulation of the  $N(x,y)$  data points (see Nielson, 1983). Pottmann extended this work to the idea of minimizing a higher degree and more general pseudonorm over the network of edges, in particular

$$\sum \int \left( \frac{\partial^3 F}{\partial e^3} \right)^2 + \text{other 3rd deriv. terms} \, ds$$

where  $e$  is in the direction of the edge and  $\tau$  normal to the edge. The solution of the minimization problem, over a suitable space of functions, is a quintic polynomial, with the first and third normal derivatives being of degree three and one, respectively. The derivatives through second order at the vertices satisfy a sparse linear system of  $5N$  equations, with the constraint that the data points must not lie on a second degree curve. The function is extended to the interior of the triangles by using a  $C^2$  blending function method. The method has quadratic precision. Some examples comparing the surface with those obtained by Nielson's method were given.

Pottmann also discussed the problem of interpolation on the sphere. He noted that the multiquadric method due to Hardy is quite successful in many cases for scattered data in the plane. On the sphere, with geodesic distance, the basis functions have a discontinuous derivative at the antipodal point. Pottmann noted that the basis function can be altered from  $\varphi(d) = \sqrt{r^2 + d^2}$  for the plane in a consistent manner for the sphere by taking the basis function (on the unit sphere) to be  $\varphi(d) = \cos^{-1}((\cos(r)\cos(d)))$ . Here  $d$  and  $r$  are geodesic distances on the sphere, or angles between the two radii to the points on the sphere. Some examples were shown.

## Interpolation of Scattered Data over Closed Domains, Tom Foley, Arizona State University (joint with D. Lane, G. Nielson, H. Hagen, and R. Franke)

Foley discussed the problem of interpolation of data defined on closed domains which are topologically equivalent to a sphere. Basically, the method is to use the mapping between the domain and the sphere (perhaps going through an intermediate rectangular parametric domain, in which case some care must be taken with poles), and then defining the interpolant on the sphere. This can be done by the use of triangular methods or methods such as variations of the multiquadric method (see Pottmann, above), or a variation of the reciprocal multiquadric method for the sphere. Additionally, if the domain is not totally specified (only points being given), the domain

may be approximated using the same method. For this, it is necessary for the domain to be star-like with respect to some point, which is taken as the center of an appropriate sphere. The domain is then a surface defined by scattered data points and is approximated by the same method. Some saving of computation accrues because the coefficient matrix for the two problems is the same. Foley's presentation was accompanied by slides illustrating various ways of visualizing a function defined on a sphere or other closed surface domains, such as: contours on the domain, radial extension "above" the domain, and perpendicular extension out from the domain (the latter two require some care to scale properly, and could give confusing or misleading impressions). For example, it is possible to combine these giving transparent surfaces for the function value with contours on the domain or the surface itself.

## Cyclide Surface Blending and Surface Modeling, Michael Pratt, Cranfield Institute of Technology

A review of cyclides and their applications in surface modeling was given. Cyclides are fourth degree surfaces and form a natural extension of quadric surfaces in that certain operations with them are closed; for example, the offset of a cyclide is a cyclide. The blending of two cylindrical pipes using cyclides was demonstrated; two cyclide pieces are needed if the centerlines of the pipes do not intersect. Blends between cones can also be constructed.

## Remarks on Cyclides in Geometric Modeling, Wolfgang Böhm, University of Braunschweig

Beginning with J. C. Maxwell's 135-year-old construction of a cyclide using "pencil and string", Böhm discussed the geometric properties of cyclides. He finished with the construction of a cyclide/spherical blend between the intersection of three mutually perpendicular circular cylinders (a tripod).

## GC<sup>n-1</sup> Functional Splines for Interpolation and Approximation of Curves, Surfaces, and Solids, Josef Hoschek, TU Darmstadt (joint with Li Jinggong, Tanji University, China, and Erich Hartmann, TU Darmstadt)

Lining curves are conic curves defined by the equation  $(1-\mu)L_1(x,y)L_2(x,y) + \mu L_4^2(x,y) = 0$  where  $\mu$  is a parameter, and  $L_1=0$ ,  $L_2=0$ , and  $L_4=0$  are lines. Such curves are easily connected with tangent continuity. Hoschek and coauthors noted that a higher degree curve of the form  $(1-\mu)L_1(x,y)L_2(x,y) + \mu L_4^3(x,y) = 0$ , enables connections with curvature continuity. Further, the process can be generalized by using a general curve  $f(x,y)$  in place of  $L_1L_2$ , and another general curve  $g(x,y)$  in place of  $L_4$ . Certain properties carry over, such as: If  $f(x,y)$  and  $g(x,y) = y = 0$  bound a convex region, the curve  $(1-\mu)f(x,y) + \mu g^n(x,y) = 0$  lies in the region for  $0 \leq \mu \leq 1$  and  $x$  lying in a suitable interval. Under suitable restrictions on the functions, the idea is also extendible to surfaces in 3-space. Patches connecting with geometric

continuity  $n-1$  can be constructed. These ideas can be used to construct blends between two surfaces.

**Spiral Arcs - An Interpolation Problem**, Harry McLaughlin, Rensselaer Polytechnic Institute (joint with Bruce Piper, RPI)

Given two points with the centers of curvature for a (proposed) curve to connect them, is it possible to construct such a connecting curve that has monotone curvature? The general answer is no; although if it is possible, the evolute of the curve plays a key role. If one extreme value is allowed for the curvature function, it is still not possible. With two extremes in the curvature function, it seems to be possible; however, inflections and cusps in the curve may occur.

**Related Topics in CAD and FEM: Isochordic Deformations**, Michel Bercovier, Hebrew University of Jerusalem

Bercovier discussed the problem of trying to represent volume preserving deformations using polynomial or rational functions. Except for trivial cases, he showed this cannot be done. Relaxing the constant volume constraint somewhat leads to a "mixed" type finite element approximation and to a solvable problem.

**GC<sup>1</sup> Conditions Between Two Rational Bezier Patches**, Dingyuan Liu, Fudan University, China

Author's abstract: The GC<sup>1</sup> necessary and sufficient conditions between two adjacent rectangular or two triangular rational Bezier surface patches are presented. Further, some practical and simple sufficient conditions are developed. There are many weights in the GC<sup>1</sup> conditions that are useful to easily compose a GC smooth surface.

**Necessary and Sufficient Conditions for Tangent Plane Continuity of Bezier Surfaces, or Tangent Plane Continuity for Bezier Surfaces - How Hard Can it Be?**, Tony DeRose, University of Washington

Author's abstract: Sets of conditions are derived that are necessary and sufficient for tangent plane continuity between two integral or rational Bezier surfaces. The patches may be given in either triangular or rectangular form, and no assumptions are made concerning the relative degrees of the patches; the only assumption is that the patches share common boundary control points (and weights in the case of rational surfaces). The conditions are shown to be minimal in the sense that they are, in general, independent.

**Supplements to the Theory of G<sup>k</sup> Continuity for Surface Patches**, Wendelin Degen, University of Stuttgart

The definition of G<sup>k</sup> continuity across patch boundaries was reviewed and compared with the notion of "contact of order k" used in differential geometry. For G<sup>2</sup> was shown that the existence of a family of curves crossing the boundary transversely with continuity G<sup>2</sup> is equivalent to both. This theory was then applied to obtain the explicit

construction of a G<sup>1</sup> join between adjacent rectangular patches, first given in implicit form by Farin (1982). Degen noted that the G<sup>2</sup> case can be handled in a similar way with an additional regularity assumption.

**Calculating Curvature Continuous Cubic Splines**, Norbert Luscher, Naval Postgraduate School

There are two nice algorithms for the computation of cubic spline curves from the B-spline control net: the deBoor algorithm and the Mansfield formula. These two methods start, respectively, from the B-spline control net and work down to the point on the curve, and start with the lower degree splines and build up to the desired degree. For splines with some tension parameters, say the  $\tau$ -splines of Böhm (1987), the algorithms do not work in the obvious fashion, although an analog of the Mansfield formula had been given. Luscher derived the analog of the deBoor algorithm in which the nice properties (such as convexity preservation) carry over. From this formulation he derived the corresponding (new and different from that mentioned) Mansfield formula.

**Piecewise Rational Curves with Frenet Frame Continuity**, T.N.T. Goodman, Dundee University

Author's abstract: A simple geometric construction is given for the Bezier points of two rational curves that join with appropriate Frenet frame continuity. This is then used to give a geometric construction, from an arbitrary sequence of control points, for the Bezier points of a sequence of rational curves of degree  $n$  that join with Frenet frame continuity of order at most  $n-1$ .

**Increasing the Flexibility of VC<sup>1</sup> Connections of Bezier Patches**, Pere Brunet, Polytechnic University of Catalonia, Spain

Author's abstract: The problem of connecting a given patch to a neighbor (to be defined) in a VC<sup>1</sup> way is studied. In practical application, we would expect some data on the neighbor to be fixed (for example, boundaries). From a counting of degrees of freedom, it can be found that this is not possible. In this sense, the algorithm of Farin '82 gives the most general solution in spite of the assumption of linearity on the coefficients of the linear combination of tangential vectors, both in the triangular and rectangular unions, and in polynomial or rational patches. After that, a method is proposed that relaxes the one-sidedness of sequential patching by modifying one control point in the data patch. The consequence is that a VC<sup>1</sup> connection with a neighbor with both endpoints completely uncoupled is always possible. Also, the modification of the data patch can be minimized.

**Fairing Bezier Curves with Some Constraints**, Horst Nowacki, Technical University of Berlin (with Dingyuan Liu, Fudan University, and Xinmin Lü, Nanjing Aeronautical Institute)

Nowacki discussed the formulation and solution of the problem of interpolation of given data with parametric

spline curves subject to an area constraint. A variational formulation was used so that the interpolant minimized the integral of the square of the  $r^{\text{th}}$  derivative (integrated with respect to the parameter). The area constraint leads to a nonlinear problem. Some examples showing the effect of various values for the area constraint were given.

**A Fast Algorithm for Raising the Degree of B-Spline Curves**, Hartmut Prautsch, Rensselaer Polytechnic Institute

It is sometimes desirable to express a B-spline curve of given degree as a B-spline curve of higher degree in order to have more flexibility available for the designer. Previous algorithms for carrying this out for degree  $n$  to  $n+1$  have required  $O(n^2)$  operations. Prautsch discussed a new algorithm for degree raising that requires only  $O(n)$  operations.

**A Rational Spline with Tension**, John Gregory, Brunel University (joint with Muhammad Sarfraz)

Gregory first developed a parametric rational cubic with a tension parameter that matched both value and slope at each of two points. At an ordered set of points, these can then be connected to give a  $C^1$  curve with local tension. By letting the slopes be unknowns and requiring  $C^2$  continuity, a system of equations is obtained, and for moderate and bigger tension values diagonal dominance accrues, hence the system has a solution. Exponential decay of the effect of tension in one interval was shown. A local basis for the curves was developed that demonstrates the usual B-spline properties of positivity, partition of unity, variation diminishing. A Bernstein-Bezier conversion is possible. With global tension values the curve tends to piecewise linear as tension gets large. Gregory calls his curves the YARBS (yet another rational B-spline), no doubt inspired by the NURBS (nonuniform rational B-splines).

**Sibson's Interpolant and Bezier Simplices**, Gerald Farin, Arizona State University

Robin Sibson (1981) defined an interesting interpolant for scattered data based upon the Dirichlet tessellation (sometimes called the Voronoi diagram, and sometimes the Thiessen polygons) with respect to the data points, and a kind of generalization of area coordinates. The approximation has some nice properties, but does not have continuous derivatives at the data points. Farin generalized this idea to obtain a smooth interpolant, cast in the form of Bezier representation, that has quadratic precision. It is easily generalized to higher dimensions. Further investigation is required to determine whether derivatives can be easily calculated, whether it can be generalized to higher degrees of smoothness, and whether it generalizes to approximation instead of interpolation.

**Finite Quadratic Segments with Conic Boundary Curves**, G. Giese, University of Dresden (joint with U. Langbecker, Berlin)

Author's abstract: For suitable segments the problem solved is how to get a representation as rational tensor product Bezier surface, which is smooth in the sense of differential geometry and which has the boundary curves as  $u$ - and  $v$ -lines. The intuitive idea of sweeping out the surface by one conic may be realized by application of known facts concerning rational Bezier representation of conics in the view of stereographic projection. The resulting representation  $x(u,v)$  is of degree  $m \leq 6$  in  $u$  and of degree  $n \leq 2$  in  $v$ . Some special problems are considered.

**Contouring Quadratics for Surface Analysis**, Andrew Worsey, University of South Carolina

Level surfaces of functions of three variables are often used for visualization and are also proposed for design purposes. It is often thought that contouring quadratic functions is easy. However, there are several problems that arise in attempting to design an algorithm for parametric quadratics (defined on a tetrahedron, say) that is robust and efficient. The contour in the faces is a quadric curve, and Worsey first finds these curves. If the contour in the face passes through a vertex, the level surface is quadratic and easily determined. If not, the level surface is a rational quartic and requires additional work. Worsey proceeds by first finding the tangent planes parallel to the tetrahedron faces to determine how the face curves are connected.

**Curvature Continuous and Convexity Preserving Interpolating Quadratic Rational Splines**, Miriam Lucien, Boeing Company, Paris

Lucien described a scheme for interpolation of a set of ordered points in the plane using rational quadratic splines that are curvature continuous. The algorithm proceeds by constructing the Bezier points from left and right toward the center simultaneously, while choosing the weights to achieve curvature continuity (in the case of an inflection point, the center of curvature flips to the opposite side of the curve, although the radius of curvature is the same). At the center, it is necessary to join the two halves in a special way to get the proper continuity, and the process depends on whether there are an even or odd number of points. The scheme preserves convexity over intervals in which the property is consistent with the data.

**Solved and Unsolved Problems in Car Body Design**, Reinhold Klass, Daimler-Benz, Sindelfingen

Klass discussed some successes and problems with the Daimler-Benz CAD/CAM system, SYRKO. Some of the problems are

- Fillets that provide a  $GC^2$  join between surfaces
- Geometric extension of curves and surfaces

- Reconstruction of surfaces from scattered data, where the surface has corners and other features
- Construction of developable surfaces to approximate the designed surface
- Rapid calculation of distance from cutter to surface of the die being cut
- Complex fillets where more than three surfaces join.

Klass finished with a conjecture: Given a surface, consider the surface obtained by an offset (distance  $r$ ) on one side. Then from this offset, an offset of distance  $2r$  back past the original surface. The final surface is an offset of the second offset of distance  $r$  back toward the original surface. Klass conjectures that this surface is the same as is obtained by using a rolling ball (radius  $r$ ) fillet (on both sides, of course).

**Topics in Bezier/B-Spline Patching of Irregular Surfaces**, Ramon Sarraga, General Motors, Warren (joint with Barbara Ericson)

Sarraga discussed an experimental system for modeling dies used to stamp automobile panels. The system necessarily involves some soft information about dies and the behavior of metal to be stamped. Starting with feature curves, an intermediate surface is defined, patch boundaries obtained, and the surface model then obtained. It is desired to use bicubic patches, so the principal problem is to build  $G^1$  bicubic patches so that the patch boundary curves are only minimally restricted.

**CASS--Computer-Aided Styling System**, Norbert Pfeiff, Volkswagen, Wolfsburg

This was a movie demonstrating the use of the Volkswagen automobile body design system--CASS.

**Multivariate Polynomial Interpolation**, Carl deBoor, University of Wisconsin (joint with Amos Ron)

The problem of polynomial interpolation of data in more than one independent variable is considerably more complicated than the univariate case. In particular, the choice of monomials, uniqueness, possible nonexistence of the interpolant, and other ideas have frustrated the would-be analyst as well as the practitioner. Given a set of (possibly scattered) data in the plane, deBoor gave a list of ten reasonable properties a polynomial interpolation set for the data should possess. Among others, these include existence, continuity (with respect to movement of the data points), scale invariance, minimal degree, monotonicity (in the sense that Newton interpolation would be possible), and inclusion of special instances; e.g., data on a rectangular or triangular grid. deBoor then defined a set of polynomials that satisfy required conditions and that yield a suitable basis set for polynomial interpolation in higher dimensional spaces.

**A Basis of  $S_{3r+1}^r$** , Peter Alfeld, University of Utah (joint with Larry Schumaker, Vanderbilt University)

**Author's abstract:** Splines (i.e., smooth piecewise polynomial functions) are used universally throughout problems involving function of one variable. It is natural to contemplate the use of similar functions in the case of several variables. However, problems that are trivial for one independent variable turn out to be extremely difficult in the case of two or more variables. In this talk, some unsolved problems concerning multivariate splines will be described and some new results will be given.

**Data Dependent Triangulations**, Larry Schumaker, Vanderbilt University (joint with Ewald Quak)

Triangulations of scattered data in the plane are usually performed to inhibit the appearance of "bad" triangles ("bad" loosely meaning long and skinny triangles). The most used and perhaps best is the Delaunay triangulation, which maximizes the minimum angle in the triangulation. This can be obtained from any other triangulation by a series of swaps of the diagonal of convex quadrilaterals that are formed by two adjacent triangles with a common edge. The diagonal is swapped if the smallest angle in the two triangles is increased. Recent work has investigated the use of alternate criteria, in particular that of choosing the triangulation that minimizes the error in the piecewise linear approximation (over the triangulation) to a given function (see Dyn). Schumaker described some experience with choosing the triangulation to minimize an energy norm for the approximating function. The energy norm is the integral (over the convex hull of the x-y data set) of the sums of the squares of the second derivatives. Since local swaps were to be performed, the process requires the specification of partial derivatives at the vertices. These were estimated from the data. The Clough-Tocher 9 parameter piecewise cubic was used to locally define the surface.

**Differential Geometry and Surface Rendering**, Rolf Walter, University of Dortmund

**Author's Abstract:** We develop a method for generating and employing contours and (self)intersections of arbitrary smooth surfaces for the purpose of visibility clarifying. The result relies on differential geometric integer invariants, called sight indices, which describe the change of visibility. These are the means to render distinguished curves like contours, (self)intersections, and boundaries, including visibility. In the same manner, but with different types of index formulas, arbitrary curves can be rendered. Also more than one surface is allowed. One advantage is that the (visible parts of) curves are drawn in one stroke. Thus, the method is especially suitable for generating high quality plots on plotters.

**Some Remarks on Convexity Preserving Interpolation**, Wolfgang Dahmen, Free University of Berlin

Beginning with data from a convex function in 2 or more independent variables, the problem is to construct a convex interpolation function for the data. It has been

shown that this cannot be done locally. It is possible to find a triangulation of the x-y data so that the piecewise linear interpolant is convex. Dahmen discussed the modification of this surface to be  $C^1$  by the analog of piecewise quadratic schemes for the one dimensional case, using the Powell-Sabin split for the piecewise quadratic triangle. The choice of center point for the split is crucial, and Dahmen observed that while it is usually possible, sometimes it is not. The extension to higher dimension using implicit piecewise surfaces that match points and normals, and in some sense preserves shape, was discussed.

**Recursive Subdivision for Curves and Surfaces**, Nira Dyn, Tel Aviv University (joint with John Gregory, Brunel University and David Levin, Tel Aviv University)

**Author's Abstract:** A family of interpolatory subdivision schemes with tension control, for the design of curves and surfaces, is reviewed. Smoothness properties of the limit curves/surfaces are discussed and the performance of the schemes is demonstrated by several pictures. In particular, the effect of the tension parameter is tested. All the schemes above are shown to be perturbations of known schemes, with the tension parameter controlling the size of the perturbation. Small positive values of the tension parameter yield a scheme that produces limit curves/surfaces with one more degree of smoothness.

**Algorithms in the Style of Böhm and Sablonniere**, Ron Goldman, Waterloo University (joint with Phillip Barry)

**Author's abstract:** The deBoor algorithm can be extended to curves that are not strictly B-splines by allowing either infinite or decreasing knots. Blossoming can then be applied recursively to these curves to compute the dual functionals of the corresponding polynomial bases. This observation leads to change of basis formulas that are the analogs of knot insertion techniques for B-splines. These methods are applied to generate transformations between the B-splines, Bezier, monomial, and power forms of a curve that are the direct analogy of Böhm's knot insertion algorithm and Sablonniere's algorithm for converting from B-splines to Bezier form.

**Symmetric Recursive Algorithms for Curves and Surfaces**, Hans-Peter Seidel, Tübingen University

The idea of a symmetric recursive algorithm was introduced, which then led to B-spline curves. The generalization to surfaces then led to the construction of a new representation for bivariate polynomials, called B-patches by Seidel. This representation has some desirable properties such as a deBoor type evaluation algorithm, easy computation of the control points, patches can be smoothly joined, and there is an algorithm for knot insertion similar to Böhm's algorithm for curves. Relaxing the symmetry conditions for the univariate case leads to ge-

ometric spline curves, and in particular it was shown that de Casteljau type evaluation algorithms exist for  $\beta$ -splines and  $\tau$ -splines.

**The Progressive Case of the de Casteljau Algorithm for Surfaces**, Lyle Ramshaw, DEC Systems Research Center

**Author's abstract:** The de Casteljau Algorithm for curves has two variants. The *plain case* evaluates a polynomial curve segment given the coefficients of its Bernstein expansion, that is, its Bezier points. The *progressive case* evaluates a spline curve given the coefficients of its B-spline expansion. It turns out that the de Casteljau Algorithm for surfaces can also be extended from the plain case to an analogous progressive case. Unfortunately, the resulting algorithm cannot be applied in any straightforward way to evaluate; e.g., a box-spline surface. Both polar forms and the symmetric variant of the tensor-product construction are useful in studying this situation.

**Almost Best Approximation of Circles by Curvature Continuous Bezier Curves**, Morton Dæhlen, Central Institute for Industrial Research (joint with Tor Dokken, CIIS, and Tom Lyche and Knut Mørken, Oslo University)

Approximation of a circular segment with angle  $\alpha$  by a cubic Bezier curve was described. The approximation was constrained to be tangent and curvature continuous, and to match such an approximation similarly when rotated through an angle  $\alpha$ . The approximation was shown to be  $O(\alpha^6)$  accurate, and a comparison with a previous method (also  $O(\alpha^6)$ ) was made, showing error about one-half as great.

**Exponential B-Splines in Tension**, Tom Lyche, Oslo University (joint with Per-Erik Koch, Trondheim University)

Splines in tension are useful for controlling unwanted behavior, such as overshoot, that occur in cubic spline curves. Lyche described the construction of a local basis for tension splines of order  $k$  with multiple knots and variable tension parameters. For small tension values, the basis functions resemble cubic splines, and as tension becomes large, approach piecewise linear functions. Knot insertion algorithms and a Bezier type representation exist. The construction gives a numerically stable basis for tension spline approximations.

**G-Splines**, Klaus Höllig, Stuttgart University (joint with Harald Mögerle)

Construction of surface approximations on rectangular patches where the patch boundaries meet in such a way that the parameter domain cannot be rectangular has long posed a problem; e.g., the corner of a suitcase. It has been shown possible to construct a  $GC^1$  surface from parametric biquadratic patches if such "corners" are isolated. Höllig showed how to construct parametric bicubic patches which give a  $GC^1$  surface.

**On Smoothness and Compatibility of Surfaces**, Jorg Peters, University of Wisconsin

Peters discussed the problems of modeling closed surfaces with parametric splines (in particular, smoothness across patch boundaries and compatibility conditions at vertices).

**Fill-in Regions for Curves and Surfaces**, Bruce Piper, Rensselaer Polytechnic Institute

Piper described an algorithm for constructing what he called a "fat curve" which approximates data described by "fat points". "Fat points" are points with some tolerance which could be a "blob", perhaps a disk or an interval (I'll just call them points from now on). Since the algorithm is geometric, various shapes can be handled. The object of the algorithm is to define a region ("fat curve") that "passes through" the given points and behaves reasonably between. "Reasonable" behavior is defined as the intersection of certain regions. For example, one being that between the two "fat" circles passing through one point on one side, and two points on the other side. The process is iterated in a certain way, decreasing the uncertainty at the given points until no improvement is attained. Now additional points are added between the existing points, and the process repeated. Eventually a "fat curve" is found that is sufficiently "thin" that the plot of it is as wide as the curve, and the process is terminated. Several examples were shown demonstrating some reasonable shapes generated from somewhat general data. The extension to surfaces defined by grids of points was discussed. The proposed algorithm is to iterate the curve algorithm in various directions on the mesh.

**Analytic, Algebraic, and Topological Properties of Plane Offset Curves**, Rida T. Farouki, IBM Watson Research Center (with Andy Neff)

Offset curves for algebraic curves of degree  $n$  are not, in general, algebraic curves, although the equation for both offset curves can be expressed as an implicit algebraic equation of degree  $4n$ . Farouki discussed the properties of offset curves from the three points of view in the title. Algebraic methods furnish an algorithmic basis for identifying all self-intersections of the offset, which are needed in order to "trim" off the resulting loop.

**Sphere-Splines with Applications**, Gregory M. Nielson, Arizona State University (joint with Randy Heiland)

The Bezier curve in the plane was generalized to a curve lying on the unit sphere by simply replacing lines by geodesics. The de Casteljau algorithm was shown to behave in the proper way and gives the algorithm for their evaluation. The Bezier representation of the analog of cubic splines (4 points per segment, curvature continuity) was obtained by solving a nonlinear system of equations for the control points. An application of the scheme to animation of a rigid object was given. Here it is necessary to interpolate a rotation matrix (the translation can

be done separately) to take on several specified positions. The constraints result in the interpolation being in 3-space and bring in quaternions. A video showing the equipment used to implement the method and some illustrative examples was shown.

**Properties and Generation of Curves to Become Boundaries of Surfaces with Prescribed Shape**, Roger Andersson, Volvo Data, Göteborg

Andersson discussed the generation of space curves for use as boundary curves in representation of automobile bodies. The behavior of the normal and binormal for such curves plays a crucial role.

**Research Directions for Curves and Surfaces**, David Ferguson, Boeing Computer Services, Seattle

Ferguson began by observing that after many years and many attempts, it is still not possible to define "fair" or "smooth" in such a way that curves and surfaces with these properties can be automatically generated. Many of the proposed solutions (such as Gordon surfaces and NURBS) do not behave as the designer wants them to, even though the mathematical properties are well known and seem very desirable. He discussed some of his experience with the topic, and software that Boeing has generated to allow an engineer or designer to obtain desired curves. The ideas underlying them is the imposition of constraints within the context of the usual curves and surfaces. For example, given some data points, the engineer may know approximately what the curve should look like. This curve may imply constraints on the value of the second derivative, and can then be imposed. In general, these kinds of constraints lead to nonlinear programming problems; however, the final results may be worthwhile. As an example, using minimum area to construct a wing-body fillet could lead to significant savings in weight of the part, which in turn leads to greater fuel efficiency.

## Conclusion

Invitations to participate in a meeting at the Mathematical Research Institute at Oberwolfach are held in high regard by the world-wide mathematical community; consequently, the meetings tend to be of very high quality. This one was no exception, with many of the well-known persons involved in the mathematics of curves and surfaces for Computer-Aided Design attending. The topics discussed included surface interrogation, interpolation, new patch definitions, geometric continuity, multivariate splines, recursive subdivision, as well as the ever-popular parametric spline curves. In this context, several new versions of spline curves were introduced, leading Tom Lyche to comment that there is always room in "the zoo of spline curves." While predominantly slanted toward the theoretical aspects of CAGD, there were presenta-

tions from those involved in the design and use of CAD systems. The CAGD community is an international one, with a great deal of research cooperation, visits to colleagues in other countries for short and long periods of time, and frequent international meetings. Consequently, it is difficult to characterize the ideas behind any particular work as having originated in Europe, the U.S., or elsewhere. I think this is a healthy situation and one that is beneficial to development of the subject.

## References

Barnhill, R.E., W. Böhm, and J. Hoschek, eds., "Surfaces in CAGD '89," North-Holland, Amsterdam, to appear.

Böhm, W., "Rational Geometric Splines," *Computer Aided Geometric Design* 4(1987)67-77.

Dyn, N., and D. Levin, "Data Dependent Triangulations for Piecewise Linear Interpolation," to appear.

Farin, G., "A Construction for Visual  $C^1$  Continuity of Polynomial Surface Patches," *Computer Graphics and Image Processing* 20(1982)272-282.

Nielson, G.M., "A Method for Interpolation of Scattered Data Based Upon a Minimum Network," *Math. Comp.* 40(1983)253-271.

Sibson, R.A., "A Brief Description of Natural Neighbor Interpolation," pp. 21-36 in *Interpreting Multivariate Data*, D.V. Barnett, ed., Wiley, New York, 1981.

# PHYSICS

## High Magnetic Field Research and Facilities III

by Dean L. Mitchell, the Liaison Scientist for Solid-State Physics in Europe and the Middle East for the Office of Naval Research European Office.

The Nijmegen High Field Magnet Laboratory (NHFML) at Nijmegen, the Netherlands, has been operational since 1976. Currently, it is one of four facilities in the world capable for user research of producing dc fields in excess of 30 tesla (T). The NHFML has five magnet stations, three of which are fitted with Bitter magnets (14.8T in a 53-mm bore, 15.2T in a 60-mm bore, and 20T in a 32-mm bore) and two with superconducting/resistive hybrid magnets (25.4T in a 32-mm bore and 30.4T in a 32-mm bore). The resistive magnets are driven by a 6-MW solid state power supply and are cooled by a closed water system that includes a 18-MWh ice reservoir supplied by refrigeration.

The NHFML occupies two floors in one wing of the physical sciences building, with the magnets and experimental stations occupying most of one floor. There is a laser and optical spectroscopy laboratory on the floor above that can be linked with the high field magnets via light pipes, optical fibers, or standard optical mirrors. The NHFML is well-equipped with the peripheral equipment which is necessary to carry out a full range of transport, magnetization, and optical measurements. The instrumentation is designed to permit experiments to be carried out over the range of temperatures from room temperature and above to 200mK. For experiments below 1K, helium-three inserts are available for the 30-T magnet. A helium-three/four top-loading dilution refrig-

erator is available for the 20-T magnet. Other special measurement facilities include: picosecond and femtosecond mode-locked laser systems; a ballistic susceptometer for the 15-T magnet; and, a specific heat calorimeter for temperatures to 1K and fields to 25T.

The laboratory is under utilized which is caused, in part, by the reduction in the inhouse scientific staff from the level anticipated when the laboratory was built. Peter Wyder, the previous director, is now director of the High Field Magnet Laboratory at Grenoble. His group was not fully replaced. The present scientific staff consists of the director, Dr. Jos Perenboom, and one other research scientist, Dr. J. Singleton. The under utilization of the facility was noted by the "Workshop on Research in High Magnetic fields" held in Nijmegen in 1987 to review "High Magnetic Field Research Programs in the Netherlands." Following the workshop, a national plan for high field facilities was developed in consultation with the Stichting voor Fundamenteel Onderzoek der Materie (FOM), which is the national support agency for fundamental research in the Netherlands. The plan recognizes the supranational roles of the dc facility at NHFML and the pulsed-field facility at Amsterdam both of which are recognized internationally. The intent of the national plan is to keep both facilities up to international standards. Initiatives have been approved to increase peak fields to 60T at the Amsterdam facility and to allow Nijmegen to in-

crease staffing to more effective levels. This staffing plan includes provisions for an additional scientist and a technician funded by FOM, a part-time chair in the Physics Department for Peter Wyder, and a future tenured faculty position in the physics department. The plan envisions an increase in the research staff to 30-40 led by 4-6 principal investigators.

Research carried out at the magnet laboratory resulted in 25 publications in 1988 with a majority involving collaborations with scientists from other institutions. These collaborations are attractive to outside users because of the relatively open scheduling that is possible at NHFML, particularly for experiments requiring long setup times or extended measurement periods.

In one series of experiments carried out by R.W.J. Hollering, NHFLM, and collaborators at the Philips Research Laboratories in Eindhoven, the energy relaxation of hot carriers in quasi-two-dimensional (2-D) AlGaAs quantum well (QW) structures were measured. Two picosecond pulses from a mode-locked dye laser were used to excite electron-hole pairs in bulk GaAs and in AlGaAs QW structures. The time and energy resolved electron-hole photoluminescent (PL) spectra were measured in fields to 25T with the sample maintained at temperature of 1.5K. The PL spectra depended both on density-of-states for the hot-carrier relaxation, and on the inelastic relaxation rates.

In a strong magnetic field, the quasi-2-D electron gas is constrained to quasi-one-dimensional motion by Landau quantization. Application of a magnetic field perpendicular to the plane of the QW thus suppresses the inelastic scattering by longitudinal optical phonons. The experiments verified a reduction in cooling rates in fields of 8T. At higher fields, the relaxation rate increased with further increases in field up to the maximum field of 20T. Theoretical calculations supported the interpretation that the suppression of local oscillator explained the reduction in the cooling rate in fields to 8T. Thereafter, the cooling rate was dominated by emission of acoustic phonons. This rate increases with increasing field. The calculations were in good agreement with the observed dependences.

The studies of relaxation processes in QW structures are important since QW devices are quite likely to operate in the hot-carrier regime where cooling rates will determine device performance.

In other studies, J. Singleton and S.J.R.M. Spermon, NHFML, collaborated with two groups at Oxford University to study the Fermi surface in the organic charge-transfer salt  $\beta''$  (BEDT-TTF)<sub>2</sub> AuBr<sub>2</sub>. The samples were prepared and characterized at Oxford. Measurement of the Schubnikov-de Haas oscillations at temperatures to 200mK and fields to 20T indicated the presence of small pockets in the Fermi surface. The magneto-resistance is highly anisotropic and anomalously

large negative values were observed for currents in the direction perpendicular to the b axis. The authors discussed and rejected the possibility that this anomaly is caused by charge-density-wave formation as observed in other charge-transfer salts. Instead, they suggested a model based on scattering from defects into open orbits. Calculations, according to the model, appeared to fit their data. This work was reported in *Physical Review Letters* 61, 2721 (1988).

If contact effects were negligible, then the two-terminal resistance for quantum hall effect devices should be the same as the Hall resistance; i.e., quantized in units of  $h/e^2$ . However, imperfect contacts, introduce corrections that typically are on the order of  $10^{-6}$ . G.L.J.A. Rikken and collaborators at NHFML, Delft University, the Netherlands, the High Field Magnet Laboratory, Grenoble, France, the Laboratory for Electronics and Applied Physics at Limeil-Brevannes, France, and the Research Institute of the German Post, Darmstadt, Germany, have made a careful investigation of these departures for gold-germanium-nickel and for tin electrodes deposited on AlGaAs metal-oxide-semiconductor field-effect transistors. The experiments relied on the use of the potentiometric resistance comparator at the Dutch National Standards Institute to compare the two-terminal resistance with the Hall resistance with a resolution of  $3 \times 10^{-8}$  or better. The results were compared with an exact theoretical evaluation valid for a junction between two isotropic media with different conductivities. Good agreement was attained for relative differences in the range  $10^{-6}$  to  $10^{-8}$ . Previous experimental studies had measured differences of this same order but were not able to determine dependences on thickness or conductivity. The significance of the present work is in the application of an exact theoretical calculation to well-defined contact configurations in order to make detailed comparisons with the experiments.

In separate work, not connected with the NHFML, L.J. Giling is developing a novel pulsed-mode reactor for low-pressure metal-organic-chemical-vapor-deposition epitaxial growth of GaAs and other compound semiconductor layers. The novelty of the reactor is the use of well-calibrated puffs to the growth substrate followed by rapid purging. In this way, the composition of the gaseous mixture at the growth interface can be independently controlled to provide a constant growth mixture, for thick layers, or a rapid change in the composition, for atomic or subatomic layers.

The MOCVD is an attractive method for growth and fabrication of planar semiconductor device structures. However, the growth conditions are difficult to model theoretically and to control experimentally. The micro-pulse capabilities of this reactor, combined with the potential for high repetition rates, may prove more tractable. Most of the work to date at NHFML has been

devoted to developing growth chambers and testing growth conditions. The reactor is now operational and

the results during the next year or so should demonstrate the usefulness of this approach.

## Workshop on Compound Semiconductor Devices and Integrated Circuits in Europe

by Dean L. Mitchell

The Workshop on Compound Semiconductor Devices and Integrated Circuits in Europe (WOCSDICE) is held annually to provide a forum for European information exchange on compound semiconductor, mainly III-V, device fabricating and processing technologies. The workshop is restricted to 60-80 participants, all of whom are expected to actively participate. Although the focus is on European work, selected individuals from the U.S. and Japan also are invited in order to provide a perspective on the status abroad. Attendees at the 1989 workshop included F. Carpasso (AT&T Bell), L.F. Eastman (Cornell), M. Heiblum (IBM), and D. Pavlidis (Michigan) from the U.S.; K. Honjo (NEC) and N. Yokoyama (Fujitsu) attended from Japan.

Dr. J. Magarshack, Thomson Hybrides et Microondes, organized the workshop as Chairman, with Dr. P.A. Rolland, the Centre Hyper-fréquences et Semiconducteurs (CHS), University of Lille, as Vice Chairman and Treasurer, and Dr. D. Lippens, CHS, as Program Chairman. The organizers and site for the workshop change each year. Recent workshops were in Lugano, Switzerland in 1988; Grainau, Germany in 1987; and Visby, Sweden in 1986. Proceedings of the workshop are not published; however, workbooks including abstracts are available to participants. In this report, I will give an overview from a semiconductor physics viewpoint and Professor Eastman will review the device technology aspects.

Research and development (R&D) in GaAs device technology is active throughout Western Europe with particularly strong efforts in France, Federal Republic of Germany (FRG), and Great Britain. The market for GaAs and other III-V semiconductor devices is small at present and mainly defense-oriented. Civilian applications are growing and major markets are projected in telecommunications and high-speed information processing. The GaAs R&D has drawn major support from the European Strategic Program for Research in Information Technology (ESPRIT) funded by the Council of Ministers of the European Community (EC). It also appears to be well-supported by the major electronic companies including Allgemeine Elektrizitäts Gesellschaft (AEG),

General Electric Company (GEC), Philips, Plessey, Siemens, and Thomson, all of whom were represented at the workshop.

The support for research on III-V semiconductor materials and devices in universities also appears quite healthy, particularly in France and the FRG. In addition to the academic and industrial research groups, France and the FRG have developed an infrastructure of research institutes that operates effectively in developing new technologies to a stage where it is practical for private industry to take over for commercialization. Notable examples are the laboratories at Bagneau and Lannion, supported by the Centre National d'Études des Télécommunications (CNET) in France, as well as the government-supported Heinrich Hertz Institut (HHI) in Berlin, and Walter Schottky Institut (WSI) in Munich.

The general topics covered by the workshop could be grouped under the three general headings of technology, devices, and integrated circuit applications with the main focus on specific device configurations.

Referring to technology, Mircea from the CNET laboratory in Bagneux, France, reviewed the use of metal oxide chemical vapor deposition (MOCVD) for large GaAs wafers. Mircea presented results on 2-inch wafers for both vertical and horizontal rotating growth pedestals. Uniformity to better than 1 percent over 2-inch wafers were attained with rotation of the wafer at 500 rpm. In fact, the measured profiles were more uniform than the computer simulation. Good uniformity also was attained with the growth of InAsP on InP. The discussion following Mircea's paper drew out the proponents of molecular beam epitaxy (MBE) who consider MOCVD to still have elements of black magic. Edge uniformity was discussed as a major problem. Atomic Layer Epitaxy (ALE) was suggested as a solution but it may not be possible to scaleup ALE to production levels required for commercialization.

A second technology that appeared to be increasingly important was using self-aligned masks to reduce stray capacitance and improve high-frequency performance. With self-aligned masks, metalized gate electrodes or

other surface features are used with beam processing techniques to provide edge alignment without using a separate mask. The consensus appeared to be that the additional processing complexity is probably only warranted for devices required in special applications.

The main theme of the workshop was the performance characteristics and limits for the device configurations and materials systems currently being produced or developed. The plan for GaAs and related III-V device technologies is to keep ahead of silicon in those applications where it has natural advantages. The advantages include high-frequency and millimeter wave oscillators, mixers, power amplifiers, detectors, and phase shifters, with applications in high-speed information processing and telecommunicating.

From the device specialist viewpoint, Les Eastman provided a stalking horse for the workshop by providing a list of the current state-of-the-art for high-speed device configurations on GaAs and on InP substrates. (See Tables 1 and 2).

**Table 1. Current State-of-the-Art for Various High-Frequency Device Configurations on GaAs Substrates**

#### MESFET

.1  $\mu\text{m}$  M gate with AlGaAs buffer  
600-700 mS/mm  $f_{\text{tx}} = 115 \text{ GHz}$   
.25  $\mu\text{m}$  gate with P GaAs buffer  
Logic gate switching < 10 ps

#### MODFET

Doped Al<sub>3</sub>Ga<sub>.7</sub>As/GaAs  
.1  $\mu\text{m}$  M gate,  $g_m = 450 \text{ mS/mm}$   
 $f_{\text{tx}} = 113 \text{ GHz}$   
.25  $\mu\text{m}$  M gate 1.8 dB noise figure at 60 GHz  
5°K noise temperature at 8 GHz (12°K)  
.25  $\mu\text{m}$  logic gates switching < 6 ps at 77K

#### SMODFET

Doped Al<sub>3</sub>Ga<sub>7</sub>As/In<sub>y</sub>Ga<sub>1-y</sub>As/GaAs  
.10  $\mu\text{m}$  M gate,  $y=.22, f_{\text{max}} = 345 \text{ GHz}, f_{\text{tx}} = 60 \text{ GHz}$   
.14  $\mu\text{m}$  M gate,  $y=.25, f_{\text{tx}} = 153 \text{ GHz}$   
 $I_{\text{DS}} = 500 \text{ mA/mm}, f_{\text{max}} = 250 \text{ GHz}$   
.25  $\mu\text{m}$  M Gate,  $y = .22, 1\text{W/mm}, 50\% \text{ power-added efficiency}$   
.25  $\mu\text{m}$  M gate,  $y = .15$   
1.6 dB noise figure at 60 GHz  
20°K noise temperature at 8 GHz (12°K)

#### HBT

1.2  $\mu\text{m}$   $5 \times 10^{17}/\text{cm}^3$  emitter,  $1 \times 10^{20}/\text{cm}^3$  base  
 $f_{\text{tx}} = 75 \text{ GHz}, f_{\text{max}} = 175 \text{ GHz}$   
Logic switching time 14 ps  
 $f_{\text{tx}} = 105 \text{ GHz}$  with ballistic electron collector

#### HBT

.25  $\mu\text{m}$  period tungsten control electrodes in base  
 $f_{\text{tx}} = 40 \text{ GHz}, f_{\text{max}} = 265 \text{ GHz}$

**Table 2. Current State-of-the-Art for Several High-Frequency Device Configurations on InP Substrates**

#### MISFET

1.0  $\mu\text{m}$  gate with SiO<sub>2</sub> insulator  
4.5 W/mm at 12 GHz, up to 45% efficiency

#### MODFET

Doped Al<sub>1.48</sub>In<sub>.52</sub>As/Ga<sub>.47</sub>In<sub>.53</sub>As/Al<sub>1.48</sub>In<sub>.52</sub>As/InP  
.2  $\mu\text{m}$  M gate -  $g_m = 800 \text{ mS/mm}$   
 $f_{\text{tx}} = 125 \text{ GHz}, f_{\text{max}} = 370 \text{ GHz}$   
.8 dB noise figure at 60 GHz  
Logic gate switching 6.0 PS @ 300 K, 4.8 Ps @ 77K  
.15  $\mu\text{m}$  M gate -  $g_m = 1320 \text{ mS/mm}, f_{\text{tx}} = 186 \text{ GHz}$   
(50  $\mu\text{m}$ )

#### SMODFET

Doped Al<sub>1.48</sub>In<sub>.52</sub>As/Ga<sub>.35</sub>In<sub>.65</sub>As/Ga<sub>.47</sub>In<sub>.53</sub>As/InP  
.10  $\mu\text{m}$  M gate,  $f_{\text{tx}} = 210 \text{ GHz}$  (200  $\mu\text{m}$ )

#### HBT

INP/In<sub>.53</sub>Ga<sub>.47</sub>As/InP - 3.6 x 3.6  $\mu\text{m}$   
Emitter doped to  $5.1 \times 10^{18}/\text{cm}^3$ , base to  $5 \times 10^{20}/\text{cm}^3$   
 $f_{\text{tx}} = 165 \text{ GHz}, f_{\text{max}} = 100 \text{ GHz}$  @ 300K  
 $f_{\text{tx}} = 244 \text{ GHz}$  at 77K

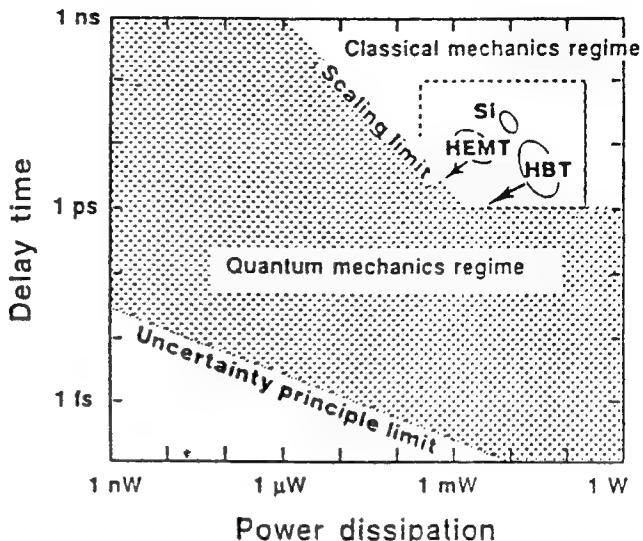
Menzel, AEG, reviewed the current status of GaAs millimeter wave integrated circuits. Menzel's survey on using monolithic Integrated Circuits (ICs) during the previous 3-4 years indicated that Schottky diodes and Metal Semiconductor Field Effect Transistors (MESFET) were the most used devices but that High Electron Mobility Transistor (HEMTs) were playing an increasingly important role. The use of Heterojunction Bipolar Transistor (HBT) devices is just beginning. Gunn diodes and GaAs impact devices also were reviewed. Newer devices, such as the strained layer Modulation Doped Field Effect Transistor (MODFETs) and quantum ballistic devices, were mentioned as potential future technologies for IC applications. An important design consideration for ICs is that the current design tools are based mainly on microstrip transmission line configurations for which computer-aided design (CAD) packages are available. Co-planar configurations have advantages; e.g., ability to provide series and shunt connections on one side of the substrate, but design tools are still limited.

The discussion of the future directions for GaAs and III-V devices centered on the reduction of critical dimensions; e.g., submicron silicon technology. An evening symposium was dedicated to tunneling and ballistic transport as related to potential device technologies. Heiblum, IBM, reviewed his studies of tunneling in device structures. The experiments were designed to help understand the physics of tunneling in such device structures rather than try to make new devices. Carpasso, AT&T Bell Laboratories, focused his review of tunneling and ballistic transport on the device implications and on

the performance characterizations that might be expected when such devices are developed in the future.

However, Yokoyama, Fujitsu Laboratories, Japan, presented the coup-de-grace. Yokoyama presented a histogram of papers at the Solid State Device meeting in Japan that carried the message that GaAs MESFETs and HEMTs are passé. Yokoyama focused his attention on HBTs and on Quantum Effect Devices (QEDs) which operate in a regime where quantum effects dominate. The regime is sketched in Figure 1, adopted from his presentation.

Yokoyama's presentation sparked an active discussion. The level of effort devoted to developing commercial devices based on quantum interference or tunneling effects is still very small in Europe. Limited research is underway in the U.S. at IBM, Bell, and perhaps two or three other laboratories directed to the development of devices. According to Yokoyama, there are five or ten programs in the major industrial laboratories in Japan that intend develop marketable devices in a near-term time scale. If true, this would indicate a particularly rapid move into commercialization since the phenomenology is still not well understood and the basic research is still concentrated in the U.S. and Europe.



**Figure 1. Delay Time as a Function of Power Dissipation for Quantum Devices with Length Scales on the Order of Electron Wavelengths**

## Workshop on Compound Semiconductor Devices and Integrated Circuits in Europe

Comments by Professor L.F. Eastman, School of Electrical Engineering, Cornell University.

### Roundtable Discussion

One highlight of the meeting was an evening round-table discussion, with audience participation, on future trends, including the role of ballistic electrons in lateral and vertical devices, the limit of frequency response in resonant tunnel oscillators, and on future quantum device limits of operations.

### Other Highlights

CNET, France, reported on large area OMVPE. Seven (two-inch) wafers were uniform (1.7 percent standard deviation in thickness) when grown at 600°C.

NEC, Japan, reported on a self-aligned H.B.T. with low oscillator phase noise. It was .6x10  $\mu$ m in emitter size, had  $f_{max}$  of 45 GHz, and had 30-40 dB less phase noise than FETs.

AEG, Germany, reported on strained-layer MODFETs with 5, 15, and 20 percent In in the InGaAs channel. The average electron velocity rose from just under  $1.6 \times 10^7$  to just over  $1.7 \times 10^7$  cm/s, for the Indium increase, at room temperature. Over  $1.8 \times 10^7$  cm/s resulted at 77K.

CNET, France, reported on InP MISFETs. They used NH<sub>3</sub> with ultra violet radiation to nitride the surface, before using UVCVD to put SiO<sub>2</sub> down at 180°C, they reported small current drifts, ion operation, of <10 percent.

CNET, France, reported on GaInP strained layers, on InP, to raise Schottky barriers. This MBE method yielded .8V barriers rather than the usual .45V barriers.

Telletra, Italy, reported on thermally activated failure in commercial MODFETs when 250°C storage tests were done up to 2500 hours.  $R_s$  rose and  $I_{dss}$  dropped 10 percent in 1600 hours, most likely a contact problem. Alu-

minimum gates and other unoptimized gates were also a problem.

Plessey, England, reported on A1,GaAs/GaAs HBT circuit applications where OMVPE was used for growth. With  $f_t = 40$  GHz, devices with  $2.5 \times 4 \mu\text{m}$  emitter areas yielded 18 dB of power at 1 GHz. Laser driver circuits and logic circuits were shown. InP emitters, with InGaAs base and collector devices, have recently been fabricated also, yielding up to 5-GHz input for divided by four circuits.

University of Lille, France, reported on experiment and theory regarding doped-channel, MIS-like FET (DMT), and MODFET. High values of breakdown resulted from the undoped A1,GaAs under the gate. With  $.5 \mu\text{m}$  gate, 48 GHz  $f_t$  and 70 GHz  $f_{\max}$  resulted.

IBM, Switzerland, reported on the role of elastic scattering on resonant tunneling. They could explain excess tunnel current by atomic steps, with  $\sim 80 \text{ \AA}$  diameter of islands of extra growth in the well or the barrier. This seems to solve this long-standing problem.

Fujitsu, Japan, reported on a wide variety of heterojunction/quantum well devices, including high current peak for current valley ratios in strained-layer AlAs/In<sub>x</sub>GaAs/InP resonant tunnel devices (over 30:1).

AEG, Federal Republic of Germany (FRG), reported on millimeter wave GaAs integrated circuits, such as 2-42 GHz distributed MODFET amplifiers.

The Technical University of Munich, FRG, reported on high frequency GaAs avalanche diodes. They got 15-W peak power from pulsed PIN devices in the 50-60 GHz range. Lower power C.W. devices had noise to signal ratios that were -86 dB, nearly as good as Gunn diodes.

The Hertz Institute, West Berlin, and SEL/Alcatel, Stuttgart, FRG, both showed heterojunction bipolar driven laser integrated circuits. Frequencies to 560 MB/s were being tested.

Siemens, FRG, showed high-speed, high-space resolution electron testing of integrated circuits.  $.5 \mu\text{m}$  spot and  $< 3.5 \text{ p.sec.}$  time resolution were reported.

Cornell University, U.S., reported new state-of-the-art results in stained-layer MODFETs on GaAs. With  $.15 \mu\text{m}$  gates,  $f_t$  of 150 GHz and  $f_{\max}$  of 250 GHz were reported.

AT&T Bell Laboratories, U.S. reported new state-of-the-art results in InP (emitter) In<sub>x</sub>GaAs (base and collector) bipolar transistors on InP. They reported 170 GHz =  $f_t$  at 200K and 250 GHz =  $f_t$  at 77K, with  $f_{\max} = 100$  GHz at 300K.

## Detonics Research and Development in France--A Discussion with General Jean Boisson, Armament Inspector for Powders and Explosives of the French Ministry of Defense

by Marco S. Di Capua, the Liaison Scientist for Physics in the Office of Naval Research European Office. Dr. Di Capua is an experimental physicist on leave from the Lawrence Livermore National Laboratory, University of California.

### Introduction

General Boisson outlined the organization of detonics research in France in the keynote address at the Third International Symposium on the Behavior of Dense Materials at High Dynamic Pressures, La Grande Motte, France in June 1989.

Boisson grouped French organizations that perform detonics research in three major ensembles--the French Atomic Energy Commission, the Ministry of Defense, and private industry. A brief description follows.

**Division of Military Applications of the French Atomic Energy Commission (CEA-DAM) (ESNIB 89-07:74-76).** The CEA-DAM performs detonics research at the centers of Limeil-Valenton (CEA/CEL-V) in the southeastern Paris suburbs, Vaujours-Moronvilliers

(CEA/CEV-M) (ESNIB 89-04:57-60) in the eastern Paris suburbs and east of Reims, Ripault (CEA/CER) near Tours and CEA-CESTA, (ESNIB 89-04:57-60) 35 km south of Bourdeaux. The activities of these centers include theory, numerical modeling, experiment, instrumentation and industrial production linked to strategic weapons. Other CEA-DAM centers are located at Bruyeres-le-Chatel (CEA/CEB3), also in the Paris suburbs and Valduc, in the vicinity of Dijon.

**Ministry of Defense Organizations.** The General Delegation for Armament (DGA) is the research, development, and procurement branch of the French Ministry of Defense. The research and development (R&D) branch of the DGA is the Directorate of Research, Studies and Techniques (DRET), which is in charge of all research upstream of development. The DRET over-

sees organizations that perform detonics R&D. One is the Central Armament Technical Establishment (ETCA) located at Arcueil. Two organizations belonging to ETCA perform detonics research. One is the laboratory at Gramat (DGA/DRET/CEG) that performs shock and blast modeling, penetration effects as well as warhead conception and evaluation. Another is the Technical Center for Testing Facilities (ETCA/CTME) in the Saclay site near Paris and a site at Captieux.

Another R&D organization attached to DRET is the French contingent of the French German Institute at Saint Louis (ISL) (ESNIB 89-03:40-43). The ISL conducts research on physics and chemistry of explosives, on detonics, and on simulation of high velocity and high pressure aerodynamic and acoustical phenomena with high explosives.

Other organizations (directorates) within DGA contract activities relating to the development and production of warheads to military industries. The role of the directorates is to finance and direct development efforts as well as to provide facilities for testing and evaluation. The Navy performs detonics research through the Directorate of Naval Construction (DGA/DCN) which maintains centers for naval weapons development--the group for studies and research in Pyrotechnics (DGA/DCN/GERP) in the Naval Arsenal of Toulon, and the group of studies, ballistic research, arms and munitions (DGA/DCN/GERBAM) at the Lorient arsenal.

Similarly, the Directorate for Terrestrial Armaments (DAT) performs pyrotechnics research through the Industrial Group of Terrestrial Armaments (GIAT) at the Tarbes (GIAT/ATS) and Salbris (GIAT/ASS) arsenals and the establishments at Bourges (GIAT/EFAB)--Etablissement Technique de Bourges and (GIAT/ETBS)--Etablissement d'Etudes et de Fabrications d'Armement de Bourges that are tasked with research, development, and evaluation of warheads for aeroterrrestrial combat. Douda (1989) describes some of these organizations in more detail.

**Industrial and Academic Organizations.** The industrial organizations are oriented mainly to the development and implementation of munitions. However, some of the establishments have the personnel and technical means to perform fundamental research through grants from the MOD.

Perhaps the first one that comes to mind is the National Corporation for Powders and Explosives (SNPE) that carries out research on explosive characterization, development of new explosives and construction of manufacturing facilities for explosives through its engineering branch SNPE Ingénierie.

Warhead development organizations such as Aerospatiale, Alsetex, Luchaire, Matra-Manurhin-Defense, the French Munitions Company (SFN), and Thomson-Brandt-Armements also perform basic research on phenomena such as jet formation, armor penetration, blast effects, and the formation and repartition of fragments.

The Research Center of the French Collieries (CERCHAR) has a group at the Verneuil installation devoted to explosive substances and safety of explosives that investigates problems related to the use of explosives in blasting applications for construction, quarries, and mines. The CERCHAR has experimental facilities to study explosions in the gaseous phase and explosions of powders.

General Boisson regretted that interest on detonics research at French universities is small. Two exceptions are a group led by Prof. Manson in the National Superior School of Mechanics and Aeronautics at the University of Poitiers, and fundamental research on explosive processes under the direction of Simone Odio at the Pierre et Marie Curie University in Paris, France.

## Summary and Conclusions

Detonics is a very lively field of R&D in France, perhaps because of a long, uninterrupted, self-reliant military tradition. Four recent symposia have had a very strong French participation--the Oxford Meeting on the Behavior of Materials at High Rates of Strain (ESNIB 89-07:35), the 11th International Symposium on Ballistics in Brussels (ESNIB 89-08:47-53), the 4th International Congress of the Working Group on Pyrotechnics, and the Third International Symposium on Behavior of Materials at High Dynamic Pressures.

## References

Douda, E.B., Report NWSC/CR/RDA-184, Naval Weapons Support Center, Ordnance Engineering Department, Crane, IN 47522-5050 (1989); and references therein.

# The Plasma Physics Laboratory at École Polytechnique, Palaiseau (Paris), France

by Dr. Marco S. Di Capua

## Introduction

The Plasma Physics Laboratory (LPMI) established at École Polytechnique in 1964, is a National Research Council (CNRS) laboratory led by Dominique Gresillon and staffed by École Polytechnique, CNRS (*ESNIB 89-07:71*), and visiting scientists from academic institutions of France and abroad. Professor Henri Doucet, the former director, is now at the French Atomic Energy Commission, Division of Military Applications (CEA-DAM) laboratory at Bruyeres le Chatel, directing the Service de Physique et Technique Nucléaire. Doucet's rotation reflects new government policies that encourage mobility in French scientific organizations (*ESNIB 89-04:67*).

The research program of LPMI explores the fundamental physics and applications of hot plasmas with some emphasis on plasmas of thermonuclear interest. Independent research teams work in the following areas:

- Nonlinear plasma physics
- Fluctuations and transport in magnetically confined plasmas
- Plasmas and beams of negative ions
- Radiation from beams and plasmas
- Atomic physics and spectroscopic diagnostics of hot plasmas
- Dynamics of plasmas.

LPMI's staff comprises 25 researchers, 6 visiting scientists, 14 staff support members, and about 13 doctoral candidates. The research staff teaches courses at École Polytechnique, directs undergraduate research projects, and supervises thesis work (even though CNRS supports a major fraction of the effort through staff positions and operational funding). A brief summary of the efforts in each area appears below.

## Nonlinear Plasma Physics

One aspect of research in nonlinear plasma physics is Anderson wave localization in plasmas. F. Doveil and S. Tsunoda, University of California, San Diego, study localized electron waves in a turbulent plasma of fluctuating density. Another research topic is the study of the nonlinear evolution of systems in the presence of simultaneous reaction and diffusion processes. Such processes occur in plasmas as well as in chemical and biological systems. H. Wilhelmsson, Chalmers Institute, Göthenborg, Sweden, has examined through a combination of numeri-

cal and analytical approaches, new solutions in such systems involving "singletons" and "polytons."

D. Gresillon and B. Cabrit have incorporated a Laser Fourier Densitometer developed at École Polytechnique into a mobile diagnostic unit to measure the turbulence developed in a supersonic flow. This system provides a measure of the turbulence (amplitudes, spectra, and propagation directions) as well as the mean velocity and temperature of the flow. The apparatus is presently installed at the high pressure, supersonic wind tunnel of the Center for Aerodynamic and Thermal Studies (CEAT), Poitiers.

T. Lehner has been modeling the formation of ionic Bernstein waves by the beat of two electromagnetic waves. Such waves, that propagate perpendicularly to the applied magnetic field in a warm plasma, could be useful as diagnostics of ionic temperature and composition and magnetic field direction in plasmas. The coupling of the waves produces a daughter wave that scatters from the induced density. An experiment to measure the scattered radiation is presently underway.

## Fluctuations and Transport in Magnetically Confined Plasmas

The École Polytechnique collaborated with the Tokomak teams of JET, Culham, U.K.; Tore-Supra, Cadarache, France; and TFR, Fontenay aux Roses, France, with measurements of energy transport and measurement of confinement losses caused by electromagnetic field fluctuations.

X. Zou and T. Lehner have proposed an experimental program to measure magnetic field fluctuations in a Tokomak by launching an electromagnetic wave across a chord of the plasma and detecting a wave that carries an imprint of the fluctuations in the plasma by undergoing mode conversion in the vicinity of the cutoff layer.

F. Gervais is heading a project that will implement an infrared diagnostic for plasma density microfluctuations in the Cadarache Tokomak based on detection of coherent diffusion of infrared radiation at two frequencies slightly shifted from one another. The Gervais team tested this technique on TFR successfully.

## Plasmas and Negative Ions Beams

The particle beam heating concept for Tokomaks has evolved towards the use of negative ions caused by the higher conversion efficiency. Negative ion sources have

evolved from surface sources to volume sources where deuterium or hydrogen ionizes in a low-pressure discharge. M. Bacal and his group developed a laser pulse technique where the pulse causes photo-detachment of an electron. A Langmuir probe measures the electron density. The technique measures the migration of H-ions into the region depopulated by the laser pulse. When the probe and the laser focal spot are not at the same location, this technique measures the ion velocity. The Doppler broadening of the spectral lines provides the ion temperature.

D. Skinner, postdoctoral fellow, University of Wisconsin, developed a model for the evolution of the ion density in the source as a function of pressure and current to explain the saturation of ion density with discharge current and the increase of ion density with pressure. The calculations show that indeed the ion density peaks for a given current and then decreases.

J. Bruneau and M. Bacal suppressed the electron current from the ion source with a magnetized region located between the source and the extraction grid. The magnetic field suppresses the electron current very effectively. The present research task is to maximize the negative ion current.

M. Hopkins, Ulster University, Northern Ireland, measured ion and electron densities in a 450- $\mu$ s pulsed source. The electron densities reach a steady state very early in the pulse while ion densities climb steadily to values that reach 70 percent of the steady state value for a source pressure of 2 mTorr. This slow climb of ion density is caused by the very slow population growth of vibrationally excited molecules.

## Radiation from Beams and Plasmas

Research on beams and plasmas pivots around the conversion of the energy of a relativistic electron beam (REB) into radiation in the mm and soft X-ray spectral ranges.

**Conversion of REB Energy into mm Waves.** The conversion of REB energy into mm waves was reported at the 10th Free Electron Laser (FEL) Conference in Israel in August 1988 (ESNIB 88-10:28 and 89-04:46; Hartemann, 1989) by F. Hartemann, Thomson-CSF, and J. Buzzi who extracted a very small fraction of a REB accelerator beam through a 1-mm diameter graphite aperture into a wiggler. To optimize the fields at the entrance region, they tapered the entrance of the helical wiggler field by a gradual reduction of current through a very ingenious copper sulphate liquid resistor. A sweep of the accelerating voltage produces microwave emission in the 75- to 180-GHz range. Buzzi measured gains of about 2.88 dB cm<sup>-1</sup> at 120 GHz. The efficiency peaks at a current of about 30 A, 0.6 MV, with a 0.96-T guide field and a 0.03-T wiggler field.

The gaussian voltage pulse waveform of the REB accelerator is inconvenient to measure FEL radiation properties such as line widths, tunability, gain, and amplifier phase stability. Hence, the group is developing an electrical power source to deliver a 1-MV, 1- $\mu$ s pulse into about 1,000 Ohms. This power source, developed in collaboration with an industrial concern, Thomson CSF-DTE, 78141 Velizy, will drive a hot cathode as the next step towards an industrial implementation of the FEL. The CEA-DAM collaborates with the electron beam diagnostics.

**Soft X-ray Production.** The production of soft X-rays revolves around the compression of Al cylindrical plasmas through magnetic forces arising from the current pulse from an REB generator. The project has two distinct flavors: (1) production and characterization of the plasma cylinder, and (2) compression of the cylinder by the self-magnetic fields.

**Plasma Production.** The plasma results from the vaporization of an 5- $\mu$ m thick Al foil in the breech of a coaxial plasma gun through a 140-kA current pulse with a 1- $\mu$ s half period delivered by a 12-kV, 500-J capacitor. Two different nozzles shape the plasma either as a 3-mm diameter cylinder or a 5 mm-thick annulus with a 1.5-cm mean radius. The 1.0E + 18-cm<sup>-3</sup> plasma cylinder exits at a 1-2-cm  $\mu$ s<sup>-1</sup> velocity.

The 1-D Lagrangian code FILM, originally developed to simulate laser plasma interactions, follows the evolution of the foil plasma assuming instantaneous heating. The simulations provide guidance on the foil geometry that will produce initial plasma conditions that are favorable for X-ray lasing after magnetic compression.

The plasma compression experiment engages P. Audibert, E. Figura, C. Rouille, and B. Etlicher with collaboration from J.P. Geindre, C. Chenais-Popovics, and J.C. Gauthier, Atomic Physics group; and A. Folkierski and S. Niffiker, Imperial College, London. A current pulse from GAEL, a water dielectric 2-Ohm, 500-kV, 250-kA pulsed-power source, compresses the plasma. The accelerator has a 50-kA prepulse that lasts about 40 ns. The current then rises to about 250 kA with a 15-ns exponential folding time. A Mach Zehnder interferometer with a 8-ns, 0.58- $\mu$  dye laser light source measures 5.0E + 18-cm<sup>-3</sup> electron densities 70 or so ns after the end of the current pulse. Filtered X-ray pinhole cameras show that the Helium-like, Raleigh-Taylor unstable, Al plasma, reaches temperatures between 200 and 250 eV.

In collaboration with CEA-DAM (ESNIB 89-04:57), plasma compression experiments with thicker shells have now begun on the 1.6-MA, 45-ns pulse AGLAE generator at the CESTA laboratory (ibid: 59). The goal is to produce a 500-eV, 1.0E + 20-cm<sup>-3</sup> collisionally excited X-ray lasing plasma.

Numerical simulation of dense Z-pinches, performed in collaboration with N. Grandjouan of the numerical analysis group uses a 0-D model (plasma conditions are uniform across the shell or cylinder) that incorporates the equations of motion, the energy equation, a QEoS equation of state (More, 1988), a radiation escape factor and electrical coupling to an external driving circuit. B. Etlicher simulated the GABEL experiment with annular as well as cylindrical plasmas with calculations that follow the plasma radius, current, temperature, electron density, plasma resistance, and the balance of joule heating, kinetic energy, pdV work, and radiated energy. The results show that a 5-mm diameter cylinder radiates about 1 kJ while a 1-cm diameter, 500- $\mu\text{m}$  thick shell with the same mass radiates only 20 J.

To simulate the AGLAE plasmas, Etlicher used a more sophisticated 1-D model that allows a radial dependence of the variables in the shell. The FILM is a cylindrical geometry, two-temperature (Te and Ti) Lagrangian code that incorporates magnetic field diffusion equations, equations of state (Sesame, QEoS, perfect gas), atomic physics, and out-of-equilibrium ionization. Atomic physics processes then determine the conductivity and the radiation history of the plasma.

The simulations of the AGLAE experiment show that a 0.1-mm thick, 1-cm radius shell, driven by a 2-MA current pulse that peaks at 60 ns, reaches the axis at 80 ns with a 2-keV temperature and a  $1.0\text{E}+21\text{-cm}^{-3}$ -electron density. Calculations reveal that current flows throughout the shell cross section, contrary to naive assumptions based upon the skin effect. The Joule and shock preheating of the inner layers can prevent the shell from reaching the desired densities at the center. Etlicher discussed these results at the Z-Pinch Workshop, June 1989, Laguna Beach, California.

These results suggest two interesting research topics: (1) the sensitivity of the radial profiles of current density to the initial conditions of the plasma in the shell, and (2) an experimental measurement of current density profiles within the imploding plasma shell to validate the calculations.

### Atomic Physics and Spectroscopic Diagnostics of Hot Plasmas

This group collaborates very actively with the group that investigates radiation from beams and plasmas in investigating the atomic physics processes that take place in Z-pinches. The research goal is to obtain plasma conditions that will support X-ray laser amplification with an ultimate goal to achieve lasing conditions in Ne-like Fe. The first step is producing and compressing Al plasma cylinders by Audebert's team as described above.

Other research involves a spectroscopic study of multi-charged ions belonging to the Ni isoelectronic series.

Spectrograph calibration with lighter elements yielded the ionization potentials of Cu- and Ni-like elements in the vicinity of Au ( $Z=79$ ) (Tragin, 1989).

N. Tragin also refined an Al tracer technique to measure the electron density and temperature of Au Ni-like ions in a Au-Al plasma mixture heated by a  $0.53\text{-}\mu\text{m}$ , 500-ps,  $1. - 5\text{E}+14\text{ W}\cdot\text{cm}^{-2}$  pulse in the LULI laser facility. The Stark broadening of the gamma line of He-like Al is the electron density diagnostic and the electron temperature results from fitting the measured intensity ratios of H-like to He-like lines using a code called SPECTRA. In principle, the electron density and temperature measured values are inputs to a collisional radiative model that calculates the level populations of Ni-like Au ions so that the intensities predicted by the calculations can be compared with the intensities measured in the experiment.

In practice, the situation is far more complicated since radiative transfer steepens the gradients of electron temperature in Au, nonstationary processes are present, and strong emission from plasma regions of lesser interest can overwhelm emission from regions where measurements are desired. Consequently, Tragin evaluated the Au plasma properties by fitting the line intensities with a computer code (HUJI), using the electron density and temperature as parameters, and justifying the value of these parameters on the basis of electron densities and temperatures measured elsewhere in the plasma or measured in different experiments (Tragin, 1989a).

C. Chenais-Popovics has elaborated on a K-alpha absorption spectroscopy technique to determine the ionic state, the electron temperature, and the areal electron density in the dense, low-temperature region of chlorinated plastic X-ray absorbing targets. A 30-J, 100-ps,  $2.0\text{E}+14 - 3.0\text{E}+15\text{ W cm}^{-2}$  laser pulse at  $0.26\text{ }\mu\text{m}$  irradiates a 0.4- to  $1.0\text{-}\mu\text{m}$  thick Bi ablator. Soft X-ray emission from the ablator heats a  $12.5\text{-}\mu\text{m}$   $\text{C}_2, \text{H}_2, \text{Cl}_2$  foil substrate.

The diagnostics include time integrated PET crystal spectrographs in the 3- to 5- $\text{\AA}$  range that view the front and rear of the target, while a time-resolved PET spectrograph views the rear of the target. Two transmission grating spectrographs and eight filtered diodes record broadband spectra in the 50-eV to 4-keV energy range. These diagnostics provide Chenais-Popovics with spatially and temporally resolved spectra from the front and the rear of the target.

In a typical experiment, Chenais-Popovics records the spectrum from the ablator front and the spectrum behind the foil substrate. The spectrum behind the substrate reveals very strong absorption lines. Neglecting self-absorption in the Bi, the difference between the spectra result from absorption by the Cl is the substrate. Absorption shifts to higher energies at higher temperatures. As an example, RELAC code calculations indicate that at 70 eV only F<sub>1</sub>, O, and N-like Cl are present, while at 190 eV

N-like Cl is barely present and absorption mainly takes place through C, B, Be, Li, and He-like Cl.

In the time resolved spectra recorded at the rear of the target, all absorption lines are present simultaneously suggesting that a temperature gradient exists in the plasma. Chenais-Popovics analyzed the data with this hypothesis, modeling the chlorinated absorber as a sequence of slabs with a monotonically decreasing temperature profile. A choice of temperature profile across the slabs provides the relative absorption at the K-edges of the successively ionized states of Cl. A choice of areal density of the absorber then matches the measured absorption in absolute value. Chenais-Popovics estimates the temperature to be 130 eV with an areal density of  $0.2 \text{ g-cm}^{-2}$  corresponding to a thickness of  $1.5 \mu\text{m}$  (Chenais-Popovics, 1988).

A refinement of this technique is deposition of a thin Al layer at successive depths in the target and to measure the K-edge absorption in this layer. This technique provides a more detailed look at the temperature distribution in the X-ray absorber (Chenais-Popovics, 1989).

## Summary

The plasma physics research effort at LPMI concentrates on a small number of very carefully chosen areas that fit closely with research efforts at French national laboratories, universities, industry, and military research organizations. The research efforts are also closely coupled with efforts abroad, especially in the area of plas-

ma diagnostics, Z-Pinches laser-matter interactions, and free electron lasers. The quality of the research staff and facilities allows LPMI to attract personnel on leave from other laboratories and personnel from LPMI appears also to be very welcome at laboratories elsewhere.

## References

Chenais-Popovics, C., et al., "Radiative Transport in a Laser Irradiated Target," *Proceedings of the 19th European Conference on Laser Interactions with Matter* (ECLIM) (1988).

Chenais-Popovics, C., et al., "K $\alpha$  Absorption Spectroscopy: Diagnostic of the Radiative Pre-Heating of a Laser-Irradiated Layered Target," *Physical Review A*, Volume 40, in press, (1989).

Hartemann, F., and Buzzi, J.M., "High Efficiency Millimeter Weave Free-Electron Laser Experiments," *Proceedings 10th Free Electron Laser Conference*, Jerusalem, Israel; submitted to Nuclear Instrumentation and Methods, 1989).

Tragin, N., et al., "Ionization Limits in Cu-like and Ni-like High-Z Ions from ab Initio Calculations and Wavelength Measurements in Rydberg Series," *Physical Review A*, Volume 39, (1989), 2085.

Tragin, N., et al., "Experimental Study of Unresolved Transition Arrays in Laser Produced Plasmas," *Proceedings of the International Congress on Optical Science and Engineering*, PMI 2136, Paris (1989a).

# NATO Advanced Study Institute on Scanning Tunneling Microscopy--Physical Concepts, Related Techniques, and Major Applications

by Marco S. Di Capua and Othmar Marti. Dr. Di Capua is the Liaison Scientist for Physics in Europe and the Middle East for the Office of Naval Research European Office. He is an experimental physicist on leave from the Lawrence Livermore National Laboratory, University of California. Dr. Marti, a former ONR postdoctoral fellow at the University of California, Santa Barbara, is a research associate at the Quantum Optics Laboratory, Swiss Federal Institute of Technology, Zurich. Dr. Marti reviewed the manuscript and provided the sections on STM in biology, imaging of surgical implants, atomic force microscopy (AFM), and AFM of biological samples.

## Introduction

This NATO Advanced Study Institute, held at the Ettore Majorana Center for Scientific Culture in Erice, Trapani, Italy, from April 17-29, 1989, covered the physical concepts of scanning tunneling microscopy (STM), related techniques, and major applications. The purpose

of this STM course was to provide a forum to deepen the understanding of the basic aspects, to identify and discuss common problems in the various applications, and to work out sound new approaches.

J. Behm, Institute of Crystallography and Mineralogy, University of Munich; N. Garcia, Universidad Autonoma de Madrid, Spain; and Nobel Laureate H. Rohrer, IBM

Research Laboratories, Zurich, organized the institute and developed the curriculum. Dr. A. Gabriele, Ettore Majorana Center, made the local arrangements. Dr. Rohrer included several graduate students and postdoctoral fellows that swelled the attendance to about 160, the maximum that Ettore Majorana Center can accommodate at one time.

The basic aspects and methods of the course covered

- Theory of tunneling
- Theory of STM imaging
- Mesoscopic quantum effects
- STM and related techniques
- Tip-surface interactions
- Metals, adsorbates, and reactions
- Semiconductor surfaces, adsorption, and epitaxy.

The related techniques covered

- Spectroscopic applications
- STM and atomic force microscopy (AFM) on liquid solid interfaces
- Imaging and conductivity of biological materials
- Point sources and collimated electrons
- Near field optical microscopy
- Force microscopy and tribology
- Surface modifications and engineering.

A background for STM techniques appeared in *Scientific American* (Rohrer, 1985) and more recent reviews on STM and related techniques appear in *Science and New Scientist* (Hansma, 1988, 1989), and *Physics World* (Gimzewski, 1989). The ESNIB reviewed the STM '88 Oxford meeting [ESNIB-88:10, (1988), 26-27 and ESNIB-89:03, (1989), 29-34]. The STM '89 was held in Oarai, Japan, July 9-14, 1989.

### Heinrich Rohrer's Remarks

At the beginning of the course, Rohrer introduced STM, a surface imaging technique, where a very sharp needle follows the contours of a surface. A feedback loop senses the electron current tunneling across the vacuum, from the sample to the tip or vice versa, and drives piezoelectric actuators that control the coordinate of the tip above the surface within a fraction of an Angstrom.

The STM imaging is a local probe with a different set of limitations from those arising from diffraction and lens aberrations in light and electron microscopy.

The STM resolution depends roughly on the square root of the product of the local tip radius (of the order of a few Angstroms) and the exponential decay distance for the tunneling current (of the order of a few Angstroms). The exponential nature of the decay of the tunneling current allows resolutions of the order of 1 Å with tips as large as few atomic dimensions and tip positioning a few Angstroms above the surface of the sample.

Rohrer then sketched very roughly, based upon his experience as a journal reviewer, a few of the pitfalls to avoid in interpreting experimental results. Among them are

- The vertical coordinate of the probe tip that maintains a constant tunneling current may not coincide with the topography of the surface, commonly defined as the surface contours of constant charge density. The tunneling current is proportional to the density of states at the Fermi energy of the atoms at the surface. Consequently, experimenters may be tempted to interpret changes in the density of states as topographical features.
- Surface deformations caused by interaction of the surface and the scanning probe are always possible. In particular, deformations caused by the interaction go unstable (Martí, 1986). Rohrer displayed topographic data for graphite where the influence of the varying repulsive forces is clearly visible (Soler, 1986). He also showed data where the attractive as well as the repulsive regimes are also visible (Martí, 1986).
- Other issues that may obscure the physical picture are when transitions from electron tunneling to point contact, or transitions from tunneling to field emission take place. In either case, the linear dependence of the logarithm of the current as a function of the tip coordinate no longer holds. Can the experimenter identify such transitions unambiguously from the data?
- Electron traps on the surface may block the tunneling current. Electrons then hop in and out of the traps changing the barrier height and causing oscillations in the current. Koch detected such instabilities three years ago (Koch, 1987). These oscillations, which can be a nuisance under some experimental conditions, can be advantageous to study electron trapping structures.
- Bistable tunneling from more than one tip location can result in imaging instabilities appearing as ghost images. This is a nuisance that experimentalists must recognize and guard against.

In a second very stimulating lecture, Rohrer reviewed some very current topics that deserved coverage by the lectures but could not be included in the program. Among the topics are:

- Photon emission with energies greater or smaller than the barrier height by adjusting the voltage of the tip accordingly.
- Detection of low energy electrons emitted with energies greater than the barrier height. These electrons can reach the detector because the applied electric field, which concentrates on the sharp tip, is quite low on the sample surface. These electrons reveal surface structures that were previously

inaccessible. A description of H.W. Fink's measurements using this technique appears below.

- Auger electrons emitted with energies greater than the incident energy that can also be used to identify underlying defects or impurities. The low-energy probing electrons produced by STM allow a much more precise localization.
- Detection of spin polarized secondary electrons that escape with zero energy from the surface (Allenspach, 1989).

Ballistic electron emission microscopy may yield great dividends in the study of the density of states and band structure at the interface of heterojunctions (Kaiser, 1988). In this technique, the STM tip faces a biased heterojunction. For voltages lower than the bottom of the conduction band energy no electrons reach the biased collector. Above the threshold voltage, the transmitted current rises linearly with the applied voltage. The spatial resolution of this technique results from two unique features: one is the collimating nature of the tunneling barrier. The other is the ballistic propagation of the electrons in the base of the junction. Hence, features lying as deep as 100 Angstroms can be revealed with resolutions of about the same dimensions.

Another exciting area is fieldless tunneling. A tip, attached to a spring, close to a surface acquires a potential that arises from the broken symmetry. In the measuring technique, motion of the spring-tip mechanical oscillator is excited at resonance by an AC voltage. The induced motion of the tip produces a large current modulation arising from the exponential dependence of tunneling current on distance. A phase sensitive detector detects when the force goes through zero and provides a direct measurement of the potential, and hence the barrier height.

Another interesting area, according to Rohrer, is scanning tunneling potentiometry (Muralt, 1987). In this technique the STM tip, excited by an AC voltage, scans across a biased heterojunction. The AC component of the resulting current signal provides a measure of the topography while the averaged component is a measure of the potential distribution across the junction.

The course had limited coverage of instrument design. Rohrer felt a few areas ought to be pointed out. Among them

- Coarse positioning of the tip on a sample is still one of the key technological issues in the application of STM, according to Rohrer. An ability to reposition the tip reproducibly at features of the surface will be essential to study the effect of *in situ* modifications. Ideally, millimeter motions of the tip in the plane of the sample would be desired, while allowing reproducible repositioning within a tenth of a micron or so. Tip repositioning hinges upon stability

of the STM instrument, and the ability to specify the coordinates of the sample where the tip will be placed.

- The stability of an STM microscope requires decoupling, through a hierarchy of natural resonant frequencies, the specimen holder from the laboratory environment, and the scanning tip from the holder. According to Rohrer, active noise control systems may improve instrument stability.
- One approach to specify coordinates is to incorporate a STM in a Scanning Electron Microscope (SEM). The SEM can rapidly scan over millimeter dimensions and returns to features that the STM explores in more detail. Rohrer cautioned, however, that an ultra-high vacuum SEM is required. Otherwise, breakdown of residual hydrocarbons by SEM electrons develops carbon insulating layers on the tip and the sample that inhibit electron tunneling.

An interesting development in the quest to sense surface features is motion of the tip in a circular pattern. Current sensors, slaved to the angular position, easily determine the topographical gradients in the surface. The tip can explore deep features in rough samples with this approach.

## Quantum Properties of Electrons in Scanning Tunneling Microscopy

The STM has sparked an interest on the quantum properties of eV energy electrons that is probably unsurpassed since the early days of atomic physics. These quantum properties can be viewed from many different viewpoints and become important when electrons interact with structures of dimensions of the order of their wavelength. The next section samples a few of these viewpoints like emission from tips, electrons "squeezing" through constrictions, interaction of low-energy electrons with solid state excitations, and revisiting some field emission issues.

## Single Atom Tips

The motivation for the production of tips that terminate in a single atom is to produce STM images with the highest possible resolution. According to Vu Thien Binh, University of Lyon, France, STM requires:

- Well-defined tips (for signal interpretation) where the position of the tunneling area, the electronic structure and the atomic arrangements are known
- Tip apex radii of less than 10 Angstroms corresponding to 1 atomic radius
- Reproducible tip fabrication with possible *in situ* regeneration.

Binh described the surface diffusion and evaporation processes that build up the tip, and the final migration of atoms, through a combination of thermal treatment and applied electric fields, that leads to a tip geometry where neighboring crystal facets meet, forming a polyhedral corner. A different process produces a pyramidal atomic cluster above a hemispherical infrastructure. Binh observed that the field emission current deviates from the linear Fowler Nordheim plot ( $\log(I/V^{**2})$  as a function of  $1/V$ ). Binh and J. Saenz, Universidad Autonoma de Madrid, believe this deviation arises because of emission from a single atom. Other participants suggested that deviation may be an artifact of the data or may have other causes associated with the physics of field emission.

J. Saenz discussed emission from tips ending at a single atom attempting to explain Binh's results. Saenz's model assumes that the microtip with a characteristic dimension of  $\sim 20$  Angstroms dominates the emission process at the lower fields. Saenz proposes that emission from the microtip saturates at the higher fields and emission from the 500 Angstroms support structure takes over. Saenz's interpretation triggered lively discussions.

W. Fink, IBM Laboratories, Zurich, discussed the incorporation of the apex atoms on the penultimate terrace of a (111) oriented tip. Field evaporation of three atoms, one at a time, produce the last terrace and the tip atom is then deposited at the center of this terrace (Fink 1986 and 1988). To deposit this last atom, Fink adjusts the flux of atoms to 1/10 of a monolayer and cycles field ion imaging and depositing to field desorb atoms in undesirable positions. One out of 10 trials resulted in a single-atom tip.

Three-atom tips emit currents as large as  $10 \mu\text{A}$ , with angular spreads of 2 degrees. One-atom tips emit with an angular spread of about 1 degree. The highest electron current for a single atom tip reported at Erice was  $1 \mu\text{A}$ .

Fink also showed that these tips produce collimated beams of electrons. By scanning samples with highly collimated electron beams from these tips and collecting secondary electrons resulting from the beam-surface interaction, Fink can extend the resolution of SEM to dimensions of a few nanometer (nm). The secondary electron emission profiles, assembled as an image, reveal features with dimensions of 5 nm (Fink, 1988).

R. Morin, CNRS Crystal Growth Laboratory, Marseille, collaborates with IBM Laboratories, Zurich, to study the nature, size, and shape of clusters on tip apexes, and their resistance to corrosion. His ultimate goal is a *blind* tip construction process that avoids field ion imaging of intermediate steps.

Morin displayed data on apex construction with alkali (Cs) atoms as an example of the experimental method. Morin observed adsorption of individual atoms by a step-wise increase of the electron emission current from the tip. When Morin compared emission from W tips and

emission from W tips covered with Cs atoms he found that the Cs apex

- Lowers the voltage required (by factors as large as 4) to reach the same emission current
- Reduces the total energy spread of the electrons, at a constant current from 0.28 V to 0.12 V
- Preserves the typical 3-degree divergence half angle for electrons.

## Electrons That Squeeze Through Constrictions of Atomic Dimensions

Electrons that squeeze through apertures of atomic dimensions not only exhibit some fascinating physics, but may be important in the production of collimated beams for STM, electron holography, interferometry, and lithography applications.

H. Deraedt, University of Antwerp and University of Amsterdam, the Netherlands (in collaboration with N. Garcia and J. Saenz, Universidad Autonoma de Madrid, Spain), described a two-dimensional, time-dependent quantum mechanical calculation for wave packets of electrons passing from a metal, through a constriction into a tunnel barrier, and then into the vacuum. The atomic dimensions of the constriction are comparable to the electron wavelength.

Deraedt's numerical simulation involves time-dependent solutions of the Schroedinger equation for the wave function of the electron packet as it squeezes through the aperture formed by an infinite potential barrier that begins at a radius greater than the radius of the aperture. Deraedt's simulations show that the properties of the tunnel barrier control the focusing of the electrons. Equipotential contours (resulting from a trapezoidal barrier) normal to the packet propagation direction favor tunneling of electrons with a large ratio of parallel to perpendicular momenta. These contours produce well-collimated, coherent packets.

The group at the Universidad Autonoma de Madrid also calculates elastic propagation of electrons through constrictions of dimensions comparable to the electron wavelength. In a letter of N. Garcia and L. Escapa (Garcia, 1989), Garcia solves the Schroedinger equation within the boundaries of two electron reservoirs connected through a constriction. The resulting conductance displays a step-wise behavior as a result of successive quantization modes that satisfy the transversal boundary conditions for the electron wave function at the constriction. The predictions of this calculation could be tested in an STM with a tip of atomic dimensions that makes a point contact with the sample. Garcia proposes that contact-sample pressure could control the dimensions of the constriction.

According to Garcia, this elastic resistance of quantum mechanical origins dominates (for small contacts) over inelastic or residual resistances and could pose severe complications in the miniaturization of devices.

E. Tekman and S. Ciraci, Bilkent University, Ankara, Turkey, also presented results of calculations of the conductance of a constriction that joins two two-dimensional electron gas reservoirs. Their calculations rely upon the quasi-one-dimensionality of the system. The basis set for the electron wave functions is a blend of two-dimensional plane waves and propagating constriction states. These states are the quantized transverse momentum states determined by the geometry and potential profile in the constriction.

In their approach, the constriction has the same effect as the one-dimensional barrier in textbook problems. Hence, it is easy to implement conventional one-dimensional techniques such as transfer matrix methods in the formalism that allow analysis of other geometries without excessive computational effort.

Their results, obtained in a PC, demonstrated that by assuming ballistic transport, it is possible to obtain quantized conductance. Resonances predicted by the calculations could be observed in experiments if the constriction could be shaped in a scale comparable to the Fermi wavelength, and the propagation through the constriction and reflections at the ends of the constriction allowed well-defined interference patterns (Tekman, 1989).

A. Yacoby and Y. Imry, Weizmann Institute, Israel, described collimation of electron beams through an analytical approach that relies upon the adiabatic approximation for electron transport in narrow constrictions. Glazmann (1988) developed this adiabatic approximation to treat constrictions that vary slowly in the direction of transport. An adiabatic process assumes that the electron conserves its transverse quantum number (transverse mode). The length scale that characterizes changes in the constriction dimensions is a smoothness parameter. Yacoby demonstrates that first order deviations from the adiabatic approximation introduce scattering into other transverse modes with a probability that is exponentially small in this smoothness parameter. Geometries that could be practically implemented reach the adiabatic limit because of this exponential dependence. Consequently, electrons that traverse an adiabatically diverging confining region (horn) undergo a large reduction of transverse momentum.

A sudden deconfinement (as in the case of a transition to free space) results in an approximate conservation of transverse momentum. Since the initial transverse momentum determines the spread of the electron beam, a horn-like geometry reduces the transverse momentum of the electrons that reach the aperture and could produce collimated beams advantageously. Such a collima-

tion effect can also take place as the electrons tunnel through the work function barrier.

## Single Electron Tunneling Effects in STM Geometries

H. van Kempen, University of Nijmegen, the Netherlands, introduced a consequence of the miniaturization of the tip-sample tunneling junction in a STM configuration. The increment of a single electron's charge in the very small capacitance  $C$  of a miniaturized tip-sample system can result in energies that are much larger than available thermal energies ( $e^{**2}/2C >> kT$ ). Theoretical calculations suggest that tunneling cannot take place unless the charge of the capacitor is more than half an electron elementary charge. Hence, the capacitance of the junction establishes a threshold tunneling voltage (so called Coulomb blockade) and an observable consequence of this effect is a deviation from the linear current voltage relation for the junction. van Bentum (1988) has observed this effect at Nijmegen. This effect will take place only in a circuit fed by a current source and does not take place in a circuit fed by a voltage source.

An even more important consequence of this Coulomb blockade is that tunneling of a single electron decreases the capacitor charge from  $+e/2$  to  $-e/2$ . Thus, the capacitor must recharge so tunneling (forbidden during the recharging interval) can take place again. Such a junction could become a coherent relaxation oscillator with frequencies equal to  $I/e$ . The current-to-frequency conversion could result in a frequency-based current standard.

One may ask how half-charges can be possible? As pointed out by Van Kampen in his lecture, a circuit has continuum properties so that a half-charge on the plate of the capacitor is possible because the other half resides elsewhere on the conductor. However, tunneling must be quantized!

This concept can be extended to an instance of an isolated particle that resides between tip and sample. This could occur when a foreign particle contaminates the tip-sample gap in an STM or in junctions purpose-built to investigate this phenomenon. The Coulomb blockade in this case produces a stepped current voltage characteristic for the junction. Each step corresponds to an additional electron on the isolated particle. Van Bentum (1988a) observed this effect in an STM-like configuration. This effect is also present in very small evaporated tunnel junctions (Fulton, 1987).

A fourth conductor added to the sample particle-tip system could act as a *control* electrode. Changes of the potential of the particle arising from the capacitive coupling of this *control* electrode can control the tunneling current with a very large voltage to current gain (very much like a field effect transistor). The speed and low dissipation of such a configuration, which could result in fast

(1.0E-12 - 1.0E-14 s) single electron logical circuits, is motivating frantic research in Nijmegen, Moscow, Gothenburg, Delft, and Bell Laboratories.

## STM Theory--Tunneling Theory and STM Image Interpretation

J. Tersoff, IBM, Yorktown Heights Laboratory, New York, discussed the theory of STM in an image interpretation context. Tersoff is acutely sensitive to the experimental basis of physical science and his viewpoint, as revealed in his lecture, is an excellent example of how theory and experiment are complementary. Tersoff framed the discussion of electron tunneling within the context of the voltage current characteristic of an interface.

Tersoff's lectures highlighted

- The difficulty in describing close surface tip interactions with a nonperturbative approach (matching wave functions across the interface). A model (jellium) that replaces the ions in the metal by a uniform positive background has been successful in some cases.
- A perturbative Hamiltonian treatment for tunneling requires the wave functions of the surface and the tip to yield the tunneling matrix elements and tunneling current.
- Modeling of the tip as a point current source (to avoid real world problems) yields a tunneling current proportional to the density of states; i.e., the charge density from states at the Fermi level at the tip position. The point source approximation is valid as long as s-waves characterize the tip.

Tersoff added the following notes of caution for theorist as well as experimentalist.

- The decay of the wave functions at large distances is important in STM calculations. Plane waves, Gaussian orbitals, or even Slater type orbitals often behave unphysically at large distances.
- Explicit integration of the Schroedinger equation is the only method that permits STM image and current calculations.
- Accurate predictions of tunneling current are suspect. The current, which is exponentially dependent on the barrier height, can change by an order of magnitude over 1 Angstrom distances.
- As the tip approaches the surface, the bare tip and bare surface wave functions overlap leading to errors in the calculation. However, in constant current (distance) imaging the error may simply become a constant multiplicative function over the whole image.
- The shape of the tip is important in the vicinity of deep structures.

- Multiple tunneling sites produce a nonlinear superposition of images that lead to confusion while preserving the periodicity of the surface.
- Tip to tip reproducibility of images is an essential requirement in STM.
- Definition of the resolution of the nonlinear STM imaging process is a tricky business. The usual concept of convolution of a measurable quantity with an instrument response function applies only in the limit of weak corrugations that allow linearization of the imaging process. Tersoff (1989) discusses these issues in more detail.
- Contamination between the tip and the surface can enhance tip-surface interactions that will easily dominate the STM imaging process. Unphysical corrugations, probably arising from tip surface interactions, have been observed in graphite and close-packed metal surface images.
- Tersoff justifiably claims that the mechanical interactions between tip and surface are one of the most important and least understood outstanding issues in STM and related microscopies.

## Tip-Surface Interactions

Tip-surface interactions are very important to STM and AFM because the interpretation of the image requires understanding the modification of the electronic and atomic structure of the sample by the tip. S. Ciraci, Bilkent University, Ankara, Turkey, in a collaborative program with the IBM Research Center, Zurich, calculates tip-surface interactions quantum mechanically.

Ciraci formulates a model where the sample and tip ions form a periodically repeating fixed lattice. Ciraci solves the three-dimensional Schroedinger equation self-consistently for the valence electrons in the lattice using tabulated pseudo-potentials that account for the presence of core electrons. The periodic repetition of the tip and the lattice allows a description of the electron by a plane wave basis set with quantum numbers (band index and propagation vector) that specify the energy of the electrons.

The calculations yield the electronic charge density, the potential, and the interatomic forces, predicting three STM operating regimes. In a first regime, the large tip-sample distance decouples the tip and the sample so the electron wave functions of the tip and the sample maintain their identity. A second regime results from the approach of the tip to the surface of the sample that lowers the potential barrier allowing the wave functions to mix, forming states that are common to the tip and the sample. Moreover, the approach of the tip to the sample breaks the symmetry of the electronic wave functions and parallel momentum is no longer conserved. Therefore, electrons can tunnel in the lowered barrier. In a third regime,

as the tip gets even closer to the sample, the potential barrier disappears locally, leading to a point contact. In this regime, the electrons no longer transport by tunneling and transport is ballistic instead.

Ciraci's calculations also reveal an attractive force between the tip and the sample at large distances that increases upon closer approach, then diminishes, goes through zero, and becomes repulsive upon very close approach between the tip and the sample. In the weak attractive regime, which corresponds to usual STM operation, the displacement of the ion cores in the tip and sample reduces the corrugations associated with the electronic charge density. These reduced corrugations lower the contrast of the STM image. In the strong attractive force region, when point contact sets in, the relation of the STM image and the electronic structure of the unperturbed sample is lost. When the strong attractive force region transitions into a repulsive force region, Ciraci's calculations reveal a substantial displacement of the ion core regions. Consequently, these calculations are very useful to predict the forces encountered by an AFM probe. One important result is that the local repulsive force at its very tip can coexist with attractive forces of the outermost probe atoms. Ciraci's results appear in a very recent series of papers (Ciraci, 1987, 1988a, 1988b, 1989a, 1989b).

## The Barrier Height in STM Imaging

A simple tunneling model yields an STM imaging current that depends exponentially on tip height:

$$J = \exp(-2kz)$$

where  $(h \text{ bar}^*k)^{**2/2^*m}$  is the work function  $\phi$ . Since the work function concept predates the development of quantum mechanics, Richard Forbes, University of Surrey, U.K., discussed the various meanings that could be and have been attached to the term work function.

The oldest concept of work function as the difference of electrochemical potential for an electron between the inside and the outside of an emitter, arose in the context of thermionic emission. A more modern concept used in surface science, according to Forbes, is the work expended to remove an electron from the Fermi level to a location *somewhat outside* the material surface. This local work function is the property of a crystal facet with a well-defined structure and applies in circumstances where there is no space charge outside the surface.

*Somewhat outside* means that the electron must be beyond the range of short range surface forces that originate with the matter-vacuum boundary and image charges. Most surface scientists would agree to this definition, even though it is not common in textbooks.

Correlation and exchange effects contribute to the local work function. The source of the correlation effect

is a charge reorganization within the surface induced by the electron outside the surface. Indistinguishability of electrons gives rise to the exchange effect. A careful calculation by Bardeen (1940) demonstrated that, at sufficient distances from the surface, the classical image force represents both effects very well.

An electric dipole layer also contributes to the local work function. This dipole layer arises from the balance of two quantum tendencies--spreading of electrons from each other, and smoothing where electrons move into recessed areas of the surface. Spreading produces a dipole with the negative end outward while smoothing results in a positive end outward. Smoluchowski (1941) demonstrated an electrostatic contribution to the work function from these two effects that depends on the crystallographic structure, changing from face to face.

Consequently, electrostatic fields known as patch fields can exist outside a neutral surface and extend into space at distances comparable to a facet dimension. These fields, according to Forbes, muddle a work function defined by removal of an electron from the Fermi level to infinity, which constitutes an average over many facets.

The above discussion shows that adsorbates, that produce a dipole layer through charge transfer between the adsorbate and the surface, can change the local work function. This phenomenon is important in electrochemical applications of STM where the tip could intrude into the dipole field of the adsorbate layer.

Close probing of a surface, with subatomic resolution techniques, will require the definition of *point work function* as an effective step height that fits a trapezoidal barrier to the actual surface potential.

Finally, Forbes echoed Tersoff by urging caution in experiments that *measure* the work function. Simple STM theory assumes a trapezoidal barrier related to the mean *point* work function. In practice, image forces and other effects described above modify the shape of the barrier and require a change of the model, like the Burgess (1953) correction in field emission theory, to yield a physical parameter characteristic of the surface. Forbes has also suggested the reviews by Dyke (1956) and Swanson (1973) as useful sources of references to older work on field emission.

## Adsorbate Characterization with STM

J. Behm, University of Munich, lectured on STM of adsorbates in a ultra high vacuum (UHV) environment. Behm demonstrated the utility of STM to reveal adsorbate modification of the substrate electronic structure and protruding electronic states of the adsorbate. As examples, Behm used substrate-adsorbate systems that exhibit peculiar qualities such as Al(111) + O, Ni(110) + O, and Ni(110) + CO. Behm reviewed the utility of

STM electron spectroscopy as a sensitive means to probe empty states and discussed some of the shortcomings of this technique in providing chemical identification of the adsorbate.

Behm then described how adsorbates distribute on surfaces using O adsorption of Ru(001) and Cu growth on Ru(001) as examples. The growth of O demonstrates how, with increasing concentrations of O, O clusters become small unstable islands, these islands form domains and finally O adsorbs statistically into the domains. The O adsorption is independent of the presence of steps in the Ru surface.

In the adsorption process of Cu, surface steps (terraces) play a fundamental role. Growth begins at the corner of the tread and riser (interior edge) of the terrace followed by condensation of Cu islands. Several layers can coexist below a threshold temperature, above which, layer by layer, growth becomes possible.

Behm's second lecture was a witness to the extraordinary quality of the images from his laboratory. The beauty of the images reflects the time-consuming, painstaking efforts expended on sample preparation. The purpose of this lecture was to demonstrate the growth of crystals and Behm used Pt(110) and Au(110) surfaces, prepared in his laboratory, as examples. The STM images display surface corrugations that compare very well with dimensions predicted by theory. In another series of images, Behm showed rearrangement of atoms in noble metal surfaces in search of energetically favorable structural arrangements. Behm also demonstrated how the topmost layer of Au(111) contracts forming features that separate hcp and fcc domains in the surface.

Images of Al(111), according to Behm, demonstrate how tip-sample interactions can lead to elastic deformations of the sample so that the STM image represents something other than the local density of states.

The STM imaging of adsorbates is also possible in ambient conditions (air) as opposed to UHV. Schardt succeeded in imaging iodine on a Pt(111) surface in air with freshly etched tungsten tips. False color images appear in the cover of the reference (Schardt, 1989).

Behm concluded his series of lectures with a demonstration of the STM technique to study surface reactions. Behm displayed a sequence of STM images in electrolyte in an experiment that begins with a clean surface, followed by Cl adsorption and desorption that returns a clean surface again. Sequential images demonstrate that the process changes the features of the surface at the atomic level. Another sequence demonstrates that step edges are very vulnerable to modification, and short range mass transport where atom rows in Pt(110) surfaces rearrange into cells in a temperature triggered transformation.

In a final sequence, he demonstrated the hydrocarbon saturation reaction (creation of double bonds) on a plati-

num catalyst. The STM follows the rearrangement of surface defects that result from the catalytic process. These structure changes begin at a step and continue at the interface of the hydrocarbon adsorbed phase.

## Spectroscopy with eV Electrons

H. van Kempen, covering another subject, described the utility of eV electrons to probe solid state excitations like phonons, magnons, and the crystal field energy levels. In this technique, an eV electron arriving from a metal at eV potentials to a metal at zero potential generates excitations. In one technique, *point contact spectroscopy*, the metals are in contact, and the incident electron scatters back to the source where it is detected. This point contact technique has provided insight, over the past 15 years, on many excitations in solids that are otherwise inaccessible.

Another technique that perhaps has a larger bearing on STM is *inelastic tunneling spectroscopy*. This technique, initially developed to study organic molecules placed in the barrier of evaporated tunnel junctions, could be used in STM-like geometries to probe the electronic, vibrational, and rotational energy levels of single molecules or even specific locations in large molecules. In this technique, the STM tip locates the molecule, and the electrons that tunnel inelastically in the neighborhood of the molecule produce excitations that kink the current voltage characteristics of the tunneling configuration. According to van Kempen, this technique is difficult to implement and success so far has been obtained in very few cases. However, van Kempen feels that this difficult research area can realize the potential of STM as a local probing tool.

The attributes of the STM as a local probing tool can be used to great advantage in characterizing high  $T_c$  superconductors. This is a very active area of van Kempen's experimental solid state physics group at Nijmegen as part of a national effort in the Netherlands.

The STM can be used advantageously as a local probe of the energy gap, a measure of the *strength* of superconductors. This gap varies locally, even in a single crystals. van Kempen, in his lecture, described alternative techniques to measure this gap showing results from Nijmegen as well as results from Volodin (1987). These results indicate that local variations of energy gap are present in crystalline high  $T_c$  superconductors in scales of a fraction of a micron.

Perhaps a more important use of STM and AFM in superconductor research is to investigate the mobility of magnetic vortices in superconductors. Their mobility gives rise to dissipation, hence finding a way to pin the vortices on lattice sites (no dissipation) is important for technological applications.

## Microfabrication and Data Storage with STM and Scanning Force Microscopy Techniques

C. Quate, Stanford University, discussed how STM and AFM techniques can record specific patterns on structures to meet a technological challenge, issued by J. Armstrong of IBM who said that a fundamental limit of 100 atoms per bit of information could be reached early next century. This challenge is based upon an extrapolation of a curve that displays the number of atoms required to store a bit of information plotted against the date of the technology. To meet this challenge, Quate said, it will be necessary to record features on surfaces about 10 atoms to a side. The Stanford group, under Quate's guidance, has set a more modest goal, maybe an area 100 Angstroms on a side that would contain 1000 atoms. The STMs and AFMs are good candidates to record, read, and erase information in scales of these dimensions.

Quate suggested that as a start, technologies used at present for storage could perhaps be adapted to an STM or AFM read-write technology; i.e., creation of electron traps in dielectric interfaces, bit-oriented optical storage in thin tellurium films and ferroelectric domains in thin films.

According to Quate, new technologies for permanent records could involve

- Writing or modifying resists with STM or AFM tips and polymerizing the modified surface to preserve the record for subsequent reading. In this instance, the resolution of the tip limits the features of the pattern as opposed to the wavelength of light in conventional or exotic lithography systems.
- Depositing metal atoms in a silicon substrate using electric fields produced by the scanning tip.
- Writing on molecular monolayers that STM can read nondestructively with lower voltages or voltages of reversed polarity.
- Attaching and detecting through STM the chemical bond particular to molecules at specific sites in the substrate.
- Denting the surface of the substrate with the tip and fixing the dents that would otherwise disappear through diffusion.
- Inducing phase transitions in metallic glasses, taking advantage of the low electron mean free path and conductivity in these materials.
- Based upon presentations of H. Guntherodt, University of Basel, another option is activation of silver halides with tunneling electrons from an STM or mechanical pressure from an AFM, chemical reduction of the Ag in the activated halide grain or crystal with a chemical developer, removing

unexposed grains with a fixer, and reading the conducting Ag clusters with STM or AFM.

Quate also described a very exciting development that will pave the transition of STM and AFM instruments from the laboratory to commercial development and industrial use. Quate fabricated 5x200x1000- $\mu\text{m}$  piezoelectric positioning actuators using standard microfabrication techniques and is presently evaluating techniques to deposit a metal tip on the actuator. Because they are small, microfabricated tips reduce sensitivity to vibration and thermal drift, thus enhancing the scanning resolution of the microscope. Moreover, since the microfabrication process is compatible with conventional integrated circuit fabrication procedures, a logical next step is integration of the signal processing circuitry and the actuator.

## Scanning Tunneling Microscopy and Electrochemistry

H. Siegenthaler, University of Bern, Switzerland, has a joint development program with IBM Laboratories, Zurich, on the application of STM in electrochemistry. The STM provides a means to investigate the local electrochemistry of a surface. Also, STM allows localization of properties that up to now were either indirectly accessible or accessible in the average. Local phenomena, which may shape the average reaction, according to Siegenthaler, are of extreme importance in electrochemistry in technologies as diverse as corrosion, rechargeable battery technology, and organic conductors.

The power of STM, according to Siegenthaler, lies in the ability to investigate local properties and electrochemical reactions simultaneously. Of course, this introduces complications such as unwanted electrochemical reactions at the tip that may change the chemical or physical properties of the tip; and modification of ionic transport to the tip or substrate caused by partial shielding by the tip geometry.

These difficulties can be overcome by controlling the electrochemistry of the tip as an electrode and reducing the effective tip area with coatings. Siegenthaler emphasized the requirement of a reference electrode that enables control of the tip and substrate reactions. This well-established control technique in electrochemistry can be extended to STM, paying particular attention to diffusion that may affect performance of the reference electrode; i.e., small distances may affect equilibration.

Results obtained so far with the STM technique are extremely encouraging. For example, it seems possible to visualize foreign monolayer formation at the electrolyte interface on conducting substrate, a critical first step in the plating process. Siegenthaler also displayed, in a nm scale, the onset of Ag(100) substrate recrystallization

along dislocations by depositing about 5 monolayers of Pb in a lead and sodium perchlorate solution.

In the future, Siegenthaler will investigation substrate reconstruction induced by monolayer adsorption. In this respect, his work is parallel to Behm's; the difference being that Behm operates in UHV and Siegenthaler operates in aqueous solution. Another area will be the investigation of organic electronic conductors in an electrolyte.

### STM in Biology

The institute devoted a whole day to biological applications of STM that ranged from DNA imaging to STM imaging of prosthetic materials and conductivity of organic molecules.

The introductory lecture was given by Dr. G. Travaglini, IBM Research Laboratories, Zurich. In the first part, he presented an account of the history of biological experiments with the STM. Nobel laureates, Binnig and Rohrer, first attempted imaging DNA (Binnig 1984). They imaged bare DNA adsorbed on a carbon film. The surprising result of those experiments was that the DNA appeared as a groove rather than a hill, a first indication of nonintuitive contrast mechanisms that are sometimes encountered in STM imaging of biological matter (see the section: Tunneling Electron Transfer Through Organic Molecules).

Travaglini then presented his work in the field, done in collaboration with M. Amrein, A. Stasiak, J. Saga, and H. Gross, the Institute of Cell Biology, ETH, Zurich. The first attempts at resolving biological materials quickly showed that it was indeed possible to do it. However, one needs a major effort in developing the appropriate preparation techniques to image biological samples under UHV conditions. The STM images of the freezedried and shaded recA-DNA complex showed the pitch and the handedness of the molecule. The STM imaging became possible only after they perfected a Pt-Ir(25%)-C coating which, unlike the standard TEM coatings, is stable without an additional C-film, has high resolution, and has a good conductivity. This experiment established a link between STM and TEM, giving confidence in the application of STM imaging of organic molecules.

In his second lecture, Travaglini focused on STM imaging mechanisms. The first STM experiments of biological matter showed an impressive amount of parameters that must be controlled. Travaglini imaged paraffin surfaces to better understand and weigh the importance of different parameters. He demonstrated that there was sufficient tunneling current to image paraffin layers 100 Angstroms thick. Sheets of paraffin molecules were resolved. C. Joachim, CNRS Laboratory for Transition Elements, University of Paris, presented, in another lecture, a theoretical model of the electron transfer mechanisms presumed to be present.

### DNA Imaging

A. Criventi, the Institute for Structure of Matter, Italy's National Research Council, presented the work of his group on the STM imaging of DNA samples. Criventi began by discussing the aberrations caused by removing water from biological samples prepared for imaging under UHV conditions such as X-ray diffraction, transmission electron microscopy, SEM, and STM in UHV.

The success of these techniques relies upon removal of the water component of biological samples. Since water is the natural environment of molecules that participate in biological processes, faithful imaging requires a technique that operates successfully in the presence of water.

As a local probe, STM is ideally suited to image immobile, conductive biological samples. Criventi's group has been successful in STM imaging of DNA molecules by endowing them with electrical conductivity and tying them to the substrate. Criventi attaches one end of a conductive organic molecule to the DNA molecule and chemically anchors the other end of the molecule to the Au substrate.

Criventi (1989) imaged (with an STM in air) samples prepared with this technique. The B type plasmid circular DNA reacted with TAPO in aqueous solution. The sample is ready for imaging after the water solvent evaporates from a drop of solution placed on a freshly prepared Au substrate.

Coarse (1 nm resolution) images reveal regularly occurring bumps with a mean spatial periodicity of 3 nm and full-width-half-maximum of 2 nm that correspond to individual spirals of the DNA helix. Higher resolution images (0.2 nm) show a fine structure within each bump that corresponds to the two backbones of DNA. The STM, operating in the barrier height mode, revealed the fine structure of the backbones. Four or five local maxima visible within each backbone are presumed to be associated with the phosphate groups.

The next step of Criventi's group is to fingerprint known base group sequences in DNA molecules; i.e., ATTATAT...or GCGCGC... Once the fingerprints of each base are known, STM sequencing of DNA may be possible.

### Imaging of Surgical Implants

As discussed by Criventi, imaging of biological molecules by STM requires some sort of attachment of the molecules to a metallic surface. Likewise, the acceptance or rejection of an surgical implant depends on some kind of bonding between the surface of the implant and body tissue; i.e., biological molecules. Emch, University of Geneva, Switzerland, studies with STM and TEM some

aspects of the interface between implants and living tissue.

The combination of STM with long scan range (up to 90  $\mu\text{m}$ ) and tip positioning facilities under an optical microscope (1- $\mu\text{m}$  repositioning accuracy) with other standard biological imaging methods has several advantages:

- Samples can be examined with known procedures and interesting locations be recorded. The locations can be found again by STM, a rare but desirable capability.
- The large scan range of their STM is essential in imaging molecules and tissue fragments in the  $\mu\text{m}$  range.
- Comparative studies with established methods will set the STM results in context with known facts.

Fibronectin molecules play a key role in the successful attachment of implants. However, the rough topography of vanadium or titanium, prepared the same way as surfaces of surgical implants, would make the image of fibronectin indistinguishable from the substrate image. So Emch reported STM imaging of the topography of fibronectin on a smooth mica substrate. A PtIr covering or Au labeling establishes sufficient conductivity for imaging.

Combined studies involving STM or AFM imaging at medium resolution like the one Emch reported are likely to be an integral part of biophysics work in the future.

### Tunneling Electron Transfer Through Organic Molecules

The understanding of tunneling electron transport through organic molecules is of great importance in understanding how organic molecules, which are nonconducting in the bulk, permit electron transfer that STM methods can image.

C. Joachim, CNRS Laboratory for Transition Elements, University of Paris, used electron tunneling in alkane chains and benzene rings as an example of tunneling processes in organic molecules. This joint project with the University of Orsay involves newly developed methods that Joachim describes as elastic scattering quantum chemistry. In this approach, Joachim links usual quantum chemistry approaches (molecular orbital calculations) with solid-state-like scattering matrix calculations for disordered systems.

Joachim models the system as a chain composed of two conductors and one molecule. He then cuts the conductor in cells and *dresses* the two last units of the cell in contact with the molecules with the molecule itself. This way he constructs an effective chain without the molecule. However, the scheme incorporates the electronic properties of the molecule through an effective Hamiltonian

which is exact as far as the electronic tunneling process through the chain is concerned.

Joachim's results show that for alkane molecules, the competition between band formation and molecular resonance shift leads to a tunneling transmission coefficient which agrees with the tunneling current measured through this molecule by Travaglini (1989). For the benzene ring, Joachim predicts electronic interference in the branches of the ring, very much like the Bohm-Aharanof effect arising from chemical substitution on the ring (Joachim, 1988).

### Atomic Force Microscopy

H. Guentherodt, University of Basel, Switzerland, gave an excellent survey lecture on AFM wherein he stressed the historical context of the AFM with earlier force measuring techniques. Guentherodt showed that the excellent work of Israelachvili (1985) answers many of the questions raised by recent AFM experiments.

The AFM, a tool for direct imaging of nonconductors with atomic resolution, is the first offspring of the STM and as such had a decisive impact on developing other scanning probe microscopes (Binnig, 1986). The heart of an AFM, like in STM, is a tip that interacts with a sample surface. The tip attaches to a spring, usually a cantilevered wire or microfabricated cantilevers. The force between the tip and the sample deflects the spring and the deflection is monitored by either tunneling, optical interferometry, or the deflection of a light beam. Any other method with a sufficient sensitivity could be employed as well.

To get a topograph of the surface, one usually scans the sample past the AFM tip with a piezoelectric translation stage. Electronic circuitry records and displays either the deflection changes of the spring (variable deflection mode) or the sample height change that maintains a constant deflection (constant force mode).

Early experiments with AFMs aimed to demonstrate the resolving power of the instrument. The imaging of the graphite surface proved the outstanding real space resolution of up to 1.5 Angstroms parallel to the surface and fractions of an Angstrom in the perpendicular direction (Binnig 1987).

Guentherodt then presented atomic resolution images of various nonconductors like molybdenum disulfide and boron nitride (Albrecht 1987). Guentherodt conducted a study of 1T-TaSe<sub>2</sub>, a material which exhibits charge density waves. The study clearly showed that AFM and STM probe different surface aspects. Whereas the STM image follows the local density of states at the Fermi level, AFM, as a zeroth approximation, probes the total charge density. In this respect, AFM images of well-ordered surfaces should be similar to the surfaces inferred from; e.g., He-scattering experiments. The AFM images of 1T-

TaSe<sub>2</sub> display the periodicity of the atomic surface structure, whereas STM display the location of the charge density waves with, at times, a superimposed atomic surface structure.

The different views of the same surface that STM and AFM provide might be of great importance in imaging biological materials. As mentioned before, there are open questions on the detailed electron transfer mechanism in these materials. Imaging of a sample both with the STM and the AFM could help distinguish the true topography in an STM picture from features resulting from a varying rate of electron transfer across the molecules.

In his second lecture, Guentherodt showed successful imaging with a variety of forces between the AFM tip and sample. With a magnetic tip (etched from a nickel wire), the AFM is sensitive to magnetic forces. The AC force detection scheme relies upon changes in the resonant frequency of the wire that result from the force fields at the surface. The magnetic AFM is able to resolve magnetic structures with a width of 200 nm. Unlike other magnetic imaging techniques, one does not have to apply developers to the surfaces under investigation.

G. Persch, IBM, Mainz, Federal Republic of Germany (FRG), showed the value of magnetic AFM to characterize the quality of magnetic coatings in a production environment. Another application of the magnetic AFM is to investigate the dependence on laser power of the bit quality in Tb-Fe thermomagnetic recording films.

In the current quest to produce high TC-superconductor materials in large quantities, Guentherodt proposed the use of magnetic AFM to study the relationship between grains, grain boundaries, magnetic flux lines and lattices and their dynamics.

Another type of force microscope detects the deflection of a tip *dragged* along the sample surface. Scans result in maps of the local friction properties (Mate, 1987).

Still another aspect of AFM is the use of the tip to produce or induce localized changes in surfaces performing a local experiment with the tip at a selected location and imaging the induced changes with the AFM. Guentherodt described an experiment where the tip applies a local surface charge. An estimate of the minimum detectable surface charge yielded about 100 electrons in an area with a diameter of 100 nm. This ability to modify the surface, and subsequently detect the modifications holds great promise for data recording at very high bit densities.

E. Schreck, University of Konstanz, FRG, described a scanning tuning fork microscope. In this microscope, the edge of a 32768-Hz quartz tuning fork from a quartz watch is approaches the surface of a sample to within a few nm. Detuning of the fork caused by the viscosity of the air cushion between the edge and the surface gets stronger as the edge comes close to the surface. The 1- $\mu$ m lateral resolution and 10-nm vertical resolution, make this microscope a good candidate to profile sur-

faces in the chip microfabrication industry. However, it must be pointed out that such a microscope only works in air.

In another presentation from the University of Konstanz, FRG, P. Guethner presented a simple AFM that employs a \$1 electric microphone (available from any electronics hobbyist's source) as the detector. The microphone membrane is the spring with a compliance on the order of 1 N/m. The built-in cavity ensures that the resonant frequency of the microphone is in the tens of kHz range. Again, this device must work in air for the microphone cavity to be effective. The microphone was built into a commercial STM. The lateral resolution of the resulting AFM is the same as that of the STM. Guethner displayed the unit cell of graphite imaged with this AFM. This setup might become a lowcost alternative for classical AFMs working in air.

## Atomic Force Microscopy of Biological Samples

P. Hansma, University of California, Santa Barbara, concentrated on the critical issues in the design of AFMs that enabled his group to perform pioneering experiments on AFM imaging and to obtain images of biological processes. Hansma reviews these issues in a recent survey article (Hansma, 1988).

Hansma showed experiments on the sample height versus force characteristics of AFMs working in air and in liquid. In a liquid, the force stays at zero until the tip touches the surface. Upon retracting, the tip sticks to the surface until a force of 1.0E-09 N is reached. An AFM in air exhibits a different characteristic--while approaching, the tip is suddenly moved towards the surface with a force of a few times 1.0E-08 N. When retracted, the tip stays in contact with the sample up to a force of 1.0E-07 N. Hansma attributes this behavior to the presence of adsorbate layers both on the sample and on the tip. When these two layers come into contact, they merge and require the 1.0E-07 N to pull them apart. Hansma's conclusion is to operate an AFM in a liquid to obtain the smallest possible forces.

These forces were essential in imaging fibrin polymerization with an AFM (Drake, 1989). The AFM that imaged the sample surface operated at a force of 1.0E-09 N in a liquid. The addition of thrombin to the liquid containing fibrinogen, triggered the polymerization of fibrinogen into fibrin strands and the subsequent connection of the strands into a net (the same reaction stops the flow of blood in a wound). Hansma recorded the time evolution of the polymerization on video tape and pointed out that this sequence of images allowed for the first time to determine that the reaction involved olygomers. An objection raised at the conference was that the presence of the AFM tip over the surface would disturb the reaction.

However, this seems not to be the case since the impulse transfer from the tip to the fibrinogen molecules is of the same order of magnitude as the impulse transmitted by red blood cells in a living environment.

Paul Hansma concluded his presentation by stating that the application of AFM to image biological processes in a molecular scale has a bright future. His results tell us why.

## Scanning Near Field Optical Microscopy

In scanning near field optical microscopy (SNOM), an antenna, which is smaller than the radiation wavelength, scans the surface of the object in close proximity. In the reflection mode of imaging, the presence of the object modulates the near field of the antenna (Fischer, 1988). In the scanning photon tunneling mode of imaging, the evanescent field of the object, which also carries sub-microscopic information, excites an antenna. The image in both modes results from the modulation, which carries information about the antenna-object distance and the optical properties of the object.

Activities in near-field microscopy began before the advent of STM using small apertures as antennas (Ash, 1972). However, the separation of the excitation and the reradiated fields, as well as the low radiation efficiency of subwavelength antennas (radiated power scales as the 6th power of size over wavelength) slowed progress considerably. However, the advent of STM technology is encouraging development in the field.

In SNOM, the antenna is the tip for a noncontact imaging technique of local optical properties. This technique can establish the topography of surfaces (conducting as well as nonconducting) and their optical properties. The latter is unique and SNOM techniques could be used in the recording and retrieving information with very high areal bit density using phase (polarizability), absorptivity, and luminescence. This technique could also be combined with nonoptical modulation techniques such as the electro- and magneto-optical effect.

The reflection imaging mode is still at the development stage by U. Fischer from Nanotec GmbH, a joint venture of Hund, and Wild-Leitz in Wetzlar, FRG. Fischer collaborates with D. Pohl at IBM Zurich Laboratories. Implementation involves microfabrication of a light source (the antenna) in which total internal reflections in a slab excite a small aperture or protrusion that acts as an antenna. A scanning device moves the object relative to the antenna, and the receiver is a conventional light microscope.

Such a setup demonstrates that SNOM can resolve lateral details as small as 30 nm and sub-nm topography details with 633-nm radiation. Fischer has also demonstrated the potential of SNOM to image differ-

ences in refractive index in the < 1 part per thousand range, to image luminescence of single molecules by exciting surface plasmons in the antenna for contrast enhancement.

The photon tunneling mode discussed by D. Courjon, CNRS Laboratory, University of Besancon, is quite similar to STM in as much as the receiving antenna is a simple etched glass tip connected to a optical fiber. Total internal reflections excite the sample. This technique is also at the experimental stage and he stresses an application to the probe near fields in integrated optics as well as microscopy.

According to Fischer and Courjon, the demonstrated resolution of this technique has not yet reached its theoretical limit, which is partly associated with the size of the antenna and can be expected to be 10 nm from spectroscopy of fluorescent molecules.

## North American Contributions

This article emphasizes the contributions of European researchers. However, the success of the institute hinged heavily on lectures of North American researchers that are well known to an American audience. These contributions were:

- A series of introductory lectures on tunneling theory by C. Leavens, National Research Council, Canada, in which he presented the theory for tunneling of electrons between semi-infinite electrodes. Leavens discussed stationary state scattering, the transfer Hamiltonian approach, elastic and inelastic tunneling, resonant tunneling in heterostructures, electron tunneling spectroscopy of electronic excitations, electron-phonon interactions in superconductors and normal metals, inelastic tunneling spectroscopy, single-electron charging effects and tunneling times. In three lectures, Leavens covered material that would fill a semester graduate course.
- A series of four lectures by R. Feenstra, IBM Yorktown Heights Laboratory, New York, on the STM of semiconductor surfaces, adsorption and epitaxy was another tour-de-force. His lectures provided a very thorough overview of state-of-the-art experiments in microscopy, spectroscopy, and spatially resolved spectroscopy. Feenstra's written lecture notes, distributed before at the start of the institute are very complete and include a comprehensive, up-to-date list of references (through early 1989). Tersoff's and Feenstra's presentations were very complementary and providing an excellent blend between theory and experiment.

## Closing Remarks

I find it difficult to convey the human touch of Heinrich Rohrer's voice as he pronounced the last words at the conference. I believe that Hein's thoughts on human strengths and weaknesses are worth repeating.

Rohrer began by telling us why he refuses to single out contributors as the most important. This process only serves to flatter the person who is called to make a judgement that may not stand the test of time.

Instead, he exhorted the participants to believe in the value of their own contributions. Such belief is essential to appreciate with generosity and without jealousy the work of others. This is the only reasonable basis for an open scientific community.

Rohrer hopes that the work on interaction microscopy (STM, AFM, ....XXM) can continue in the style of the last 8 years even though the community has grown remarkably, and proprietary and even genetic engineering applications loom in the horizon. Rohrer urged the participants to stop occasionally to take a view of their doings making sure that their science agrees with their conscience. The brain is often wrong, but the heart is never wrong.

## References

Albrecht, T.R., and Quate, C.F. "Atomic Resolution Imaging of a Nonconductor by Atomic Force Microscopy," *Journal of Applied Physics*, Vol. 62, (1987), 2599-2602.

Allenspach, R., et al., *Applied Physics Letters*, Vol. 54, (1989), 587.

Bardeen, J., "The Image and Van der Waals Forces at a Metallic Surface," *Physical Review*, Volume 60, (1941), 661-674.

Binnig, G. and Rohrer, H., *Trends in Physics*, (1984).

Binnig, G., et al., "Atomic Force Microscope," *Physical Review Letters*, Vol. 56, (1986), 930-933.

Binnig, G., et al., "Atomic Resolution with Atomic Force Microscope," *Europhysics Letters*, Vol. 3, (1987), 1281-1286.

Ciraci, S. et al., "Scanning Electron Microscopy at Small Tip to Surface Distances," *Physical Review B*, Volume 36, (1987), 6194.

Ciraci, S., et al., "Scanning Tunneling Microscopy and Atomic Force Microscopy of Graphite Including Tip Surface Interaction Effects," *Journal of Vacuum Science and Technology*, Volume A6, (1988), 313.

Ciraci, S., et al., "Effect of Tip Profile on Atomic Force Microscopy," *Physical Review Letters*, Volume 60, (1988b), 1314.

Ciraci et al., "Tip Sample Interaction Effects in Atomic Force Microscopy," submitted to *Physical Review B* (1989).

Ciraci et al., "Tip Induced Modifications in Scanning Tunneling Microscopy Images," submitted to *Physical Review Letters* (1989).

Cricenti, A. et al., "Molecular Structure of DNA by Scanning tunneling Microscopy," submitted to *Science* (1989).

Drake, B. et al., "Imaging Crystals, Polymers and Processes with the Atomic Force Microscope," *Science*, Volume 243, (1989), 1586-1589.

Dyke, W. P. et al., "Field Emission," in: *Advances in Electronics and Electron Physics*, (Academic Press, NY, 1956, 89-185).

Fink, H.W., *IBM J. Res. Dev.*, Volume 30, (1986), 430.

Fink, H.W., "Point Sources for Ions and Electrons," *Physica Scripta*, Volume 38, (1988), 260-263.

Fischer, U., et al., "Near Field Optical Scanning Microscopy in Reflection," *Applied Physics Letters*, Volume 52, (1988), 249-251.

Fulton, T. A., "Observation of Single Electron Charging Effects in Small Tunnel Junctions," *Physical Review Letters*, Volume 59, (1988), 109-112.

Garcia, N., et al., "Elastic Oscillatory Resistance of Small Contacts," *Applied Physics Letters*, (1989) (in press).

Gimzewski, J., "New Fields for STMs," *Physics World*, Volume 2, Number 7, (1989), 25-28.

Hansma, P., et al., "Scanning Tunneling Microscopy and Atomic Force Microscopy: Application to Biology and Technology," *Science*, Volume 242, (1988), 209-216.

Hansma, P., et al., "Microscopes with a Feel for Molecules," *New Scientist*, Volume 122, Number 1666, (1989), 52-56.

Israelachvili, J.N., *Intermolecular Forces*, (Academic Press, NY, 1985).

Joachim, C., *Chemical Physics Letters* (1988).

Kaiser, W.J. et al., "Direct Investigation of Subsurface Interface Electronic Structure by Ballistic-Electron-Emission Microscopy," *Physical Review Letters*, Vol. 60, (1988), 1406-1409.

Marti, O. "Scanning Tunneling Microscope at Low Temperatures," Dissertation ETH Zurich No. 8095, (1986).

Mate, C.M. et al., "Atomic-Scale Friction of a Tungsten Tip on a Graphite Surface," *Physical Review Letters*, Vol. 59, (1987), 1942.

Muralt, P. et al., "Scanning Tunneling Microscopy and Potentiometry on a Semiconductor Heterojunction," *Applied Physics Letters*, Vol. 50, (1987), 135.

Schardt, B., "Atomic Resolution Imaging of Adsorbates on Metal Surfaces in Air: Iodine Adsorption on Pt(111)," *Science*, Volume 243, (1989), 1050-1052.

Smoluchowski, R., "Anisotropy of the Electronic Wave Function of Metals," *Physical Review*, Volume 60, (1941) 661-674.

Swanson, L.W. et al., "Recent Advances in Field Electron Microscopy of Metals," *Advances in Electronics and Electron Physics*, Volume 32 (1973) 193.

Tekman, E., et al., "Novel Features of Ballistic Transport through a 1-D Constriction," *Physical Review B*, Volume 39, Number 11 (1989).

Tersoff, J., *Physical Review B*, Volume 39, (1989), 1052.

Travaglini, G. et al., *Zeitschrift fur Physik* (1989), in press.

van Bentum, P.J.M., et al., "Single-Electron Tunneling Observed With Point-Contact Tunnel Junctions," *Physical Review Letters*, Volume 60, (1988), 369.

van Bentum, P.J.M., et al., "Incremental Charging of Single Small Particles," *Physical Review Letters*, Volume 60, (1988a), 2543.

Volodin, A.P. et al., "Scanning Tunneling Spectroscopy of a Microcrystal of the High-Temperature Superconductors  $YBa_2Cu_3O_{6+y}$ ," *JETP Lett.*, Volume 46, (1987) 588-591.

Williams, N. E., *Journal of Ultrastructure Research*, Volume 25, (1968), n 271.

## Fourth International Workshop on Computational Condensed-Matter Physics: Total Energy and Force Methods

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### Introduction

I traveled to Trieste, Italy, to participate in the Fourth International Workshop on Computational Condensed-Matter Physics: Total Energy and Force Methods, and to initiate a collaboration with the group of Car and Parrinello at the International School for Advanced Study (SISSA). First, the most noteworthy advances presented at the workshop are discussed, then I will describe the various research projects and problems addressed during my 1-week stay at SISSA.

### Workshop on Total Energy Methods

This workshop series was initiated about 8 years ago primarily by Volker Heine, Cavendish Laboratories, Cambridge, to establish a European forum in electronic structure theory and to stimulate European efforts in this important area.

In Braunschweig in 1984, I presented an invited talk at the second workshop in this series and it is clear from the comparison between the two workshops that the European efforts have grown very strongly over the past 4 years. The workshop itself has become more international in character, with increased international participation and both a European chairman (M. Scheffler, Fritz Haber Institute) and an American (A.R. Williams, IBM Watson Research Center). The next workshop will also

be in Trieste (January 1991). The European chairman will be R. Car (SISSA, Trieste), while the American chairman will be M. Schlüter (AT&T Bell Laboratories). In part, because of the success of this workshop, a limited participation American workshop on computational methods is being organized by D. Ceperley and R. Martin at the University of Illinois, during the week preceding the APS March Meeting.

The substantial workshop activity attests to the vitality of this research area. In fact, the methodology of computational methods has entered into a phase of rapid growth, which, together with the advances in computer capacity, is likely to lead to dramatic advances in our ability to explain and predict the properties of real materials from computer calculations. I expect this period of growth to last at least 5 years, during which this research area will remain rather "hot." I will describe specific highlights of the workshop from a personal perspective and explain their significance.

**Extensions of Density Functional Theory.** Density functional theory forms the theoretical basis for most of the present-day understanding of real materials. The local version of this theory is used in almost all band structure calculations and in many cluster and molecular calculations. However, local density theory fails in the description of strongly correlated systems involving localized spins; e.g., mixed valence compounds, magnetic impurities in nonmagnetic hosts in the nondilute limit,

and the new superconductors. However, since the density functional theory correctly takes into account the "average" exchange and correlation contributions as well as charge transfer and self-consistency effects, it can be used to obtain self-consistent, *ab initio* parameters that would enter simplified many-body hamiltonians. These hamiltonians can then be used to describe the many-body effects that are not correctly accounted for in density functional theory. O. Gunnarsson (Max-Planck, Stuttgart) and R. Martin (University of Illinois) have described applications of this technique to Mn impurities in CdTe, CdS, and ZnO, and to high- $T_c$  superconductors, respectively.

The application to magnetic impurities via the Anderson model showed that both atomic relaxation and charge transfer effects between the impurity and the host are important, and good agreement between the calculated widths of the d-bands and the experiment was obtained. The application to the superconductors used a constrained local spin density formalism to calculate matrix elements important for the various proposed mechanisms of high- $T_c$  superconductivity. One should mention that the constrained local spin density (LSD) formalism results in very good ionization energies for atoms when compared with experiment. For the solid, the calculations were carried out by identifying a relevant localized state, and then calculating; e.g., an electron-electron repulsion parameter while removing some of the interactions with the host, thereby not allowing the orbital to rehybridize. These calculations predict a very large electron-electron repulsion parameter for the copper d-electrons (8.5 eV), which is as big as the width of the O p-band. This value, which is corroborated by independent calculations of Hybertson and Schluter, basically rules out a mixed-valence copper mechanism for superconductivity. Other parameters were calculated as well and mixing between copper d and oxygen p states was found to be substantial. Needless to say, since even the simplified hamiltonian is very difficult to solve and the uncertainty in some of the parameters is substantial, no conclusions about the mechanism of superconductivity can be drawn at present from these calculations. However, the comparison of the results with present and future experiments will help in either confirming the plausibility or ruling out various proposed mechanisms.

**Quantum Monte Carlo Methods.** Another fault of present-day density functional methods is the overestimation of binding in calculations of cohesive energies. One should stress here that the exact density functional method must give the correct groundstate energy of the system, but the local density version of the density functional theory typically overbinds by 0.5-1 eV per atom, even when some nonlocal corrections are included. It is not known at present how to improve the local density theory, but another approach, the so-called quantum

Monte Carlo method, was recently shown to work for at least one important class of solids, namely diamond and graphite.

At least two versions of quantum Monte Carlo techniques exist. In the first method, the variational Monte Carlo technique, a given wavefunction ansatz is used in variational calculation of the ground state energy. The second method, Green's function Monte Carlo, is capable of generating an exact answer provided that enough sampling points have been used. The recent breakthrough in the applications of Monte Carlo techniques came with the development of methods to use *ab initio* pseudopotentials, rather than the true Coulomb potentials, in Monte Carlo calculations. This is because in the Monte-Carlo-type methods, the convergence properties are strongly Z-dependent and the use of pseudopotentials eliminates the core electrons from the calculations. S.G. Louie, University of California, Berkeley, discussed his breakthrough calculations of the cohesive energies of diamond and graphite. These calculations, which were variational in nature, reproduced the experimental values within 0.1 eV. Louis has also applied this method to the Ni atom and obtained very good results.

Although the results are extremely promising, there is some skepticism regarding the general applicability of this methodology, because the success of the variational approach depends critically on the correct choice of the basis functions. In this case, a single Slater determinant formed from local density wavefunctions was used. This determinant was augmented with a Jastrow factor and another single-body term. However, in a complicated problem, the choice of the variational basis may be far less obvious. These methods could not be generalized to the Green's function Monte Carlo approach because of the method of handling the nonlocal pseudopotential developed by the Berkeley group.

A pseudopotential formalism suitable for Green's function Monte Carlo calculations was presented by Mitas, Bachelet, and Ceperley. Previous "exact" Monte Carlo results for atoms were reproduced with this formalism and the same procedures can be applied to solids. However, this new, local pseudopotential has very strong short-range components and may require an order of magnitude more stringent convergence criteria.

**The Band Gap Problem and Self-Energy Corrections.** The Density Functional Theory (DTF) is a groundstate theory, and as such does not describe correctly the excitation properties of a system; e.g., the semiconductor band gaps. This is a very well-known problem that has been addressed successfully during the past few years with the so-called GW (Green's function width dynamical screened coolant interaction) approach, where the full many-body hamiltonian is solved to first order in self-energy using the local density wavefunctions as a basis set. For semiconductors and insulators, this method has

worked very well and reproduced all the major band gaps within 0.1 eV. M. Hybertson, AT&T Bell Laboratories, has applied the method to more complicated systems, such as surfaces, and found that the occupied states are reproduced within 0.1 eV and the surface gap with 0.2 eV. However, these types of calculations are computationally very heavy, tripling the time of the usual local density approximation (LDA) surface calculations. Hybertson then described an approximation scheme which would reduce the expense of the calculations, but the success of this approximation turned out to be problem-dependent. Therefore, there is presently no accurate alternative to the band gap problem a part from full-scale quasi-particle or quantum Monte Carlo calculations.

R. Goodby, Cavendish Laboratories, addressed the problem of the "exact" density functional theory by calculating the metallization point of Si in the diamond structure within the GW approximation and within DFT where the "exact" exchange-correlation potential was derived from the quasiparticle energies. Goodby found that the density functional theory did not give a correct metallization point. If correct, this result would have wide-ranging consequences because DFT is expected to reproduce the groundstate properties exactly. However, Gunnarsson pointed out that the exchange-correlation potential in a model system may be poor even when the band gaps are good, thereby casting doubt on the validity of the procedure used by Goodby.

**Ab Initio Molecular Dynamics.** V. Heine stated in this closing address that perhaps the most perceptive trend throughout the workshop was the gradual shift towards ab initio molecular dynamics methods, all stimulated by the famous Car-Parinello paper. Indeed, several new and important results were presented and several other presentations contained ab initio molecular dynamics as a high priority item on their "to do" list.

The ab initio molecular dynamics method, often called the Car-Parinello method, involves a simultaneous electronic structure and molecular dynamics calculation, in which the forces on the atoms are calculated via the ab initio local density method. The present implementations of this technique mostly follow the Car-Parinello paper, in which a plane wave basis is used. The relevant system, be it a cluster, a disordered solid, or an impurity in a semiconductor, is studied in a large, periodically repeated supercell. The reasons for the use of plan waves stems from the fact that the kinetic energy is diagonal in reciprocal space, while the potential energy is diagonal in real space. The transformations between the two representations are carried out using Fast Fourier transform algorithms, and result in an overall  $N \log N$  scaling for smaller calculations, where  $N$  is the number of plane waves. Larger calculations scale as  $n^2 N$ , where  $n$  is the number of occupied states, but in both cases this method

is substantially faster than traditional electronic structure techniques, which scale as  $N^3$  even for static calculations.

The applications discussed at the workshop included studies of the structure of amorphous and liquid carbon, hydrogen diffusion in silicon, the structure and properties of chalcogen molecules, and transformation of point defect structures in GaAs. Most of the presented results would be almost impossible to obtain using traditional electronic structure methods and represent major firsts for any material. This is because many of the calculated properties like the high temperature diffusion constants or the structure of an amorphous material require either a time-dependent simulation or a search for a global minimum, which is also best carried out using molecular dynamics techniques.

Apart from the results specific to systems under study, a few general conclusions stand out:

- The Car-Parinello method has indeed proven itself as a method of choice for most local density based calculations for main group elements and compounds, be it solids or clusters.
- Realistic time-dependent studies of supercells containing up to 100 atoms are possible on today's supercomputers, but the simulation times are rather short; i.e., up to about 10,000 timesteps, which corresponds at best to 100 molecular vibrations.
- The method needs substantial generalizations before it can be applied to large transition metal systems. One should mention in this context two posters: (1) Pederson, Harrison, and Klein (Naval Research Laboratory, Washington, D.C.) have developed a floating guassian Car-Parinello-type method; and (2) P. Ballone (Cornell University) and G. Galli (University of Illinois) found a convenient way to test the convergence of various approximation methods by expanding transition metal diatomics in a set of cylindrical waves of energies up to 100 Ry.

**LMTO Methods.** The Linear combination of muffin-tin orbitals (LMTO) method is an all-electron band structure method that uses only one or two sets of s, p, and d orbitals per atom to achieve a remarkable degree of accuracy for bulk metals. It has been first developed, along with the better-known linearized augmented plane wave (LAPW) method, by O.K. Andersen and collaborators. The LMTO method is very fast computationally and has been applied to many complex systems; e.g., the calculation of the many-body parameters for the new superconductors was carried out using this method. However, the standard LMTO method employs a muffin-tin approximation which makes it unsuitable for studies of low symmetry systems, such as surfaces, or for high accuracy calculations of structural parameters that are needed for ab initio determination of phase diagrams.

At the workshop, three separate implementations of the full potential LMTO method were described--all include non-muffin-tin terms in the potential. The applications ranged from interface calculations for silicides to studies of lattice dynamics of perovskites. I believe that this development is quite significant, since the LMTO approach can handle complicated transition metal compounds that present a challenge for pseudopotential-based techniques.

**Approximate Total Energy Methods.** Several problems require calculations of total energies of a cluster or supercell too large for ab initio calculations. These problems can be approached by atomic effective potentials. Accurate effective potentials are also needed for large-scale molecular dynamics simulations and for semiquantitative analyses. In the past couple of years, there has been rapid progress in this area and good effective potentials have been developed for metals, using the effective medium and embedded atom techniques; and for semiconductors, using functions which explicitly include covalent three-body terms.

At the workshop, Norskov, Denmark, reviewed his effective medium and the closely related embedded atom methods and discussed recent applications to melting of Al surfaces. For static calculations, the results agreed within 3 percent with experiments and the more accurate LAPW calculations. In general, the embedded atom and the common implementations of the effective medium method are accurate for fcc metals, while the description of bcc metals requires correction terms. These terms are somewhat cumbersome and would substantially slow down molecular dynamics simulations.

Kaxiras, IBM T.J. Watson, described a new effective potential for Si, which improved substantially the description of the total energy surface for the direct exchange mechanism for self-diffusion in Si. The formation energies of other defect structures were also described well, but not the energetics of high pressure phases. It remains to be seen whether the use of this potential will lead to a substantially better accuracy than other potentials in describing the growth of Si or the dynamics of self diffusion.

## Visit to the SISSA

Following the workshop, I spent one week at SISSA visiting R. Car. The purpose of the visit was (1) to establish collaborative efforts with the Car-Parinello group, (2) to obtain a working knowledge of their latest codes for ab initio molecular dynamics simulations, and (3) to learn about various yet unpublished techniques and procedures for performing large-scale Car-Parinello simulations. During my stay, I also met several other scientists working at SISSA, including S. Baroni, F. Ercolessi, A. Selloni, and A. Tossati. I have also interacted with

several students, some of whom I may attempt to recruit as postdoctoral associates when they obtain their degrees.

Overall, I was very impressed with the theoretical solid-state effort in Trieste, which is at par with the best institutions in Europe. Together with the International Center for Theoretical Physics (ICTP) and the University of Trieste, there are about 30-40 professional theorists employed in the area. A strong graduate student program has also been established.

The ICTP provides many workshops and conferences during the year and has a very active visitors program, which also enhances the scientific atmosphere. Since the ICTP is operated by UNESCO, many of the visitors are from Third World countries, but workshop organizers and invited speakers are generally well-known scientists of international caliber from the West.

Both SISSA and ICTP are expanding; a new building is being constructed for SISSA, while an addition to the ICTP building will double the existing space. The scientists at SISSA appear also very well equipped, with latest models of DEC workstations and both satellite- and ground-links to the Italian supercomputer center at Bologna. The Bologna Center has a Cray 1 and a Cray X-MP/408 with a VAX 8800 front end, as well as an IBM 3090/VP. There are also some indications that a Cray YMP will be added shortly to this rather impressive line-up. At present, additional equipment is being supplied to SISSA by IBM and the SISSA scientists will also have access to the latest model Convex minisupercomputer that will be installed at ICTP.

Two versions of the Car-Parinello codes presently exist at SISSA. A fast real version is being used for the majority of the simulations. This version employs the Kleinman-Bylander pseudopotentials and is only used with one  $k$ -point, namely the point. The Kleinman-Bylander pseudopotential speeds up substantially the calculations of the nonlocal contributions, while the use of the point ensures that the wavefunctions remain real. This version has been used with supercells containing up to 128 atoms, but the number of plane waves per atom had to be relatively small for the largest supercells. The experience of the group with this program suggests that for applications to liquids and disordered systems, the plane wave cutoff (which determines the number of plane waves) must be large, while the use of only the point does not affect the results. For calculation of defect  $\Gamma$  properties and probably for surfaces, a more accurate  $k$ -space integration and/or the use of a very large supercell was more important than the number of plane waves. For clusters, one  $k$ -point is of course sufficient, since there should be no  $k$ -space dispersion in the energy levels if the supercell is sufficiently large. In practice, one can use other  $k$ -points in order to check the convergence for a given supercell size.

The complex version of the program is three times slower than the real one per  $k$ -point and uses the Bachelet

pseudopotentials. However, it allows for the use of any  $k$ -points in the calculations, which is important for solids. This version has been used for supercells of up to 64 atoms.

During my stay in Trieste, I used both versions and carried out test simulations for several systems, including small Al clusters and Si and GaAs supercells. The purpose was to gain experience, rather than to achieve specific results. In order to save computer time, most of the runs involved eight or fewer atoms and relatively low cut-offs. Upon the completion of my visit, I took a magnetic tape with both the programs and the test results with me, in order to help in the implementation and optimization of the programs on our computers.

The technical aspects I discussed with Car were the various implementations of the ab initio molecular dynamics algorithms and their efficiency. In particular, two aspects of the simulations demand attention. One is the simulation of metallic systems, where the gaps between the electronic states near the Fermi level are so small that energy is transferred between the ions and the electrons during high temperature simulations. After a few hundred steps, the electrons leave the Born-Oppenheimer surface and the electronic subsystem must be cooled by several electrons-only steps. This difficulty is expected to occur in only the largest clusters, since in the smaller ones the gap between the occupied and unoccupied states will be as large as in semiconducting systems, where this problem does not occur.

The second aspect is related to achieving convergence in the fastest possible manner during geometry optimization and simulations. For geometry optimization, several methods have been proposed and implemented by vari-

ous groups. The experience of the Trieste group is that the conjugate gradient type methods converge fastest, and Car described a particular implementation of this method that is adapted to the molecular dynamics with electronic and ionic degrees of freedom. This method is yet to be implemented into Trieste codes, although it has been tested at IBM Zurich. Other methods converge slower and/or lead to other difficulties. In particular, the Trieste group found that the "diagonally dominant" method proposed by Joannopoulos and coworkers diverges or oscillates for disordered and possibly other systems.

At the risk of becoming too technical, I should mention that during my testing there, I discovered an instability associated with iterative orthogonalization of electronic wavefunctions during molecular dynamics simulations in some of the systems I was studying. This problem can be avoided in geometry optimization problems by using noniterative methods, but the iterative method must be used in simulations in order to ensure a correct time development of the system. We have not yet found the origin of this difficulty and are continuing to work on it. Other problems which we have addressed included calculations of free energy differences by ab initio methods and optimization for long-time simulations of large systems.

I found the visit to Trieste to be very important for the future research plans of my group. My only regret is that I could not allocate more time for the visit, since I was trying to accomplish in a week what took a month for all the previous visitors. I will continue to collaborate with Car.

## PSYCHOLOGY

### Influence of the Minority on the Majority

by Dr. William D. Crano, formerly the Liaison Scientist for Psychology in Europe and the Middle East for the Office of Naval Research European Office from June 1986 through August 1988. He returned to Texas A&M University, where he is a Professor of Psychology. Currently on leave of absence, he is Director of the Program in Social Psychology, National Science Foundation, Washington, D.C.

The focus of the 3rd workshop on minority influence, University of Perugia, Italy, June 22-24, was the influence of the minority on the majority. Seventeen papers were presented at the workshop, by participants from France, Switzerland, Federal Republic of Germany, Greece, Italy, England, Spain, and the U.S. The workshop was

supported by the European Association of Experimental Social Psychology and the University of Perugia.

Although issues of minority group influence have been part of the European psychology scene for more than two decades, very little research is evident in American psychological and sociological journals. Therefore, research on minority group influence is relevant, and potentially

enlightening, for American behavioral scientists. This is not to say that American social research has ignored persuasion-related topics. Indeed, from its very beginnings as a scientific discipline, American social psychology has been concerned with the process(es) of social influence. However, with some notable exceptions (e.g., Clark & Maass, 1988; Nemeth & Wachtler, 1973; Nemeth, Wachtler, & Endicott, 1977; Maass & Clark, 1983, 1984, 1986), in much American research, the effect of minority influence on the majority has been ignored. The thrust of the seminal work of Sherif (1936) on norm formation, for example, and of Asch (1951), which focused on the manner in which respondents were "brought into line," with a majority opinion, has been carried forward even into today's research (cf. Crano, 1970, 1975, 1978; Crano & Messe, 1982). Hence, the research presented in this workshop is not only pertinent, but novel for American audiences.

Reaction of European psychologists to our one-sided preoccupation with minority influence has not been favorable. Indeed, the emphasis on the subjugation of the minority by the majority struck many Europeans as symptomatic of the inequities of American society. In his powerful critique of American social influence research, Serge Moscovici, cohost of this workshop, suggested the American overemphasis on majority influence was shortsighted and wrong-headed--to ignore minority influence is to ignore the impact of such deviants as Freud, Einstein, Marx, and Christ. Moscovici (1976) and his colleagues (e.g., Moscovici & Mugny, 1987; Mugny & Perez, 1986) sought to demonstrate the power of the minority to change orthodox opinion. In so doing, they greatly enlarged our conception of social influence.

There can be no doubt that the minority can influence the mainstream--just as there can be no doubt that minorities oftentimes have no impact whatsoever. Several explanations for the manner in which minority groups work their will on the majority, and the conditions under which such influence attempts succeed or fail, will be discussed in the following paragraphs. But before beginning with a formal presentation of some of the research discussed in Perugia, let me first provide a general overview of minority influence research.

## Processes

Moscovici, Ecole des Hautes Etudes en Sciences Sociales, Paris, argued that when a person is confronted with a message that argues for a position that varies from his, one of his first responses is to determine the source of the disagreement. If the source is representative of the majority group, a central motive is to bring oneself into line with the majority. Majority influence activates a relatively shallow process in which one's own opinion is com-

pared with that of the majority, and the perceiver attempts to incorporate the new (majority) information with his. Theoretically, people find it comforting to be included among the majority on most issues.

However, when faced with a disagreement from a minority group member, "the main preoccupation is to see what the minority sees, to understand what it understands" (Moscovici, 1980, p. 25). Such a process has some interesting implications. First, it suggests that disagreement with a minority group representative will stimulate more divergent, creative thinking than will disagreement with a majority group representative. Research by Nemeth, University of California, Berkeley, reported at this conference and elsewhere (e.g., Nemeth & Kwan, 1985, 1986) supported these expectations. It also suggests that minority influence might take some time to manifest itself; i.e., a certain amount of cognitive work must take place before one can resolve the conflict brought about by the minority. Again, there is ample support for this possibility, as shown in the work discussed by Mugny, University of Geneva, Switzerland, at this conference.

## Paradigms

The study of minority influence has been carried out through the use of several research paradigms, each of which is focused on different forms of response. For example, in the standard attitude change paradigm, research subjects are asked to express an opinion on a topic, and then are provided with a counter-attitudinal communication, ascribed either to a majority- or a minority-group member. Effects of majority- and minority-group influence agents on immediate and delayed attitude change typically are measured in this paradigm.

In the divergent or creative thinking research of Nemeth and her colleagues, subjects are put in a learning situation, and then are confronted with the apparently inappropriate answers of a majority- or minority-group person. Effects of such a treatment on subjects' resultant thought processes are the central issue of such an approach.

In yet another form of minority influence study, subjects are asked to make a perceptual judgment in concert with an experimental confederate whose characteristics obviously label him as a member of the majority, or a minority group. Effects of the confederate's attempts at influencing the perceptions of the naive subject are measured immediately, in the presence of the confederate, and again after the confederate and, typically, after the confederate has been removed from the scene. Some exceptionally interesting results have been derived from this paradigm, and it is to this perceptual research that we will first turn our attention.

## Minority Influence on Perceptions

One of the most extraordinary findings in the study of minority group influence was produced by Bernard Personnaz (1981). In this three-phase study, subjects first were to judge the color of a light projected onto a screen. (Most people perceive the light as blue, although it is close to the perceptual border between blue and green.) Subjects responded in concert with an experimental confederate, who was described as belonging either to the majority or to a minority group. The confederate saw the light as being green. Interesting differences were observed in the session in which both subject and confederate were responding together. When the confederate was presented as a majority member, he successfully changed the subjects' responses. Conversely, when the confederate was presented as a minority group representative, he had no apparent influence on subjects' responses.

In a second section of the experiment, the experimenter asked the subjects to fixate on the light and write their answers. No one but the experimenter, presumably, was privy to the answers. Thus, in this "private" response condition, the confederate would not know the subjects' responses and the influence of the majority group confederate dropped off considerably.

Most interesting are the results of the third phase of the experiment. Subjects again were to fixate on the light, but were asked (again in private) to report the perceptual afterimage that they saw once the light had been extinguished. In such a circumstance, we see the complement of the color presented. So, for example, if we fixate on a red light, and then turn to a white background, we perceive a green perceptual afterimage; if an orange light is shown, we see a blue afterimage.

An extraordinary finding was discovered in this phase of Personnaz's study. The subjects who had been exposed to the majority confederate, and who were induced to report the light as being green (consistent with the majority group confederate's response, but probably contrary to their true perceptions) reported an orange afterimage which would be perceived if the primary stimulus were perceived as blue. This suggests that subjects in this condition of the experiment who responded consistently with the confederate did not really see what they reported.

However, subjects paired with the minority group confederate, and who were not influenced (at least in public) by his responses (and thus, who continuously responded "blue" despite the confederate's apparent perceptions of green), reported afterimages that tended toward red, the complement of green. In other words, the subjects paired with the minority group confederate were privately influenced by his reports (they saw green). They were very reluctant to allow this influence to be made public, and as such, reported seeing blue, which they knew to be the perception of the majority of subjects. The stunning aspect

of this work is that it suggests that fundamental perceptual processes can be socially influenced.

Since it is extremely unlikely that most subjects knew what the perceptual afterimage of a blue or green light was, it is also unlikely that these findings were the result of suspicious subjects, experimenter bias, or the host of other complicating factors. As such, even if subjects wanted to fake an appropriate response, they probably would not know how.

Bernard and Marie Personnaz, University of Paris, France, discussed some conceptual replications of this work at this conference. In one of these replications, female subjects were paired either with an attractive or unattractive female confederate (actually, the same confederate, but dressed and madeup differently to suit the experimental occasion), who consistently reported seeing green, when the majority reported seeing blue. In phase one, subjects were most influenced publicly by the attractive confederate; but her impact faded when she left the situation in phase two. When not present physically, the attractive confederate had almost no impact on subjects' perceptions of the afterimage. The opposite results were found with the unattractive confederate.

Although no direct influence was apparent in phase one, in phase two the unattractive confederate had considerable impact on subjects' perceptions of the afterimage. The Personnaz used social comparison theory (cf. Festinger, 1954) to explain their results. This theory holds that when objective means of comparison are unavailable, we compare ourselves with others to determine the validity of our views. We find it threatening to compare ourselves with others who are considerably more talented or attractive than ourselves. Accordingly, reasoned Personnaz, the attractive confederate would be influential in the direct influence conditions, but would prove somewhat threatening over the long term, and ultimately her influence would be rejected. The unattractive confederate would not be a person with whom the subject would wish to identify, and hence her influence would be minor in the *public* response condition. However, since the unattractive confederate would not prove threatening, her influence (which was present in the *public* response condition, but resisted) would apparently grow when she was physically removed, and the subject was to form judgments alone. Results consistent with these expectations were reported.

## Creativity Enhancement by Minority Opposition

As noted, Nemeth's work suggests that minority groups stimulate divergent, creative thought. The outcome of a test of this hypothesis was discussed by Anne Maass and Chiara Volpato, University of Padua, Italy. In their research, high school students from Milan were

asked to respond to a report, apparently prepared by other highschoolers, which argued for tougher college entrance examinations. The report was allegedly a minority position, and had been prepared either by a group of Milanese students (an ingroup minority, since the subjects were Milanese too) or by a group of Roman high school students (an outgroup minority). Consistent with their expectations, Maass and Volpato found that when subjects were asked to accept or reject the proffered solution, or to create their own, those paired with the ingroup minority; i.e., fellow Milanese students, were much more likely to attempt to generate new, alternative solutions. In explaining this result, they argued that ingroup minorities stimulate the kind of divergent thought processes hypothesized by Nemeth, thus leading to creating a new solution. The outgroup minority (Roman students) did not stimulate creative thought processes; subjects either agreed or disagreed with their position on the desirability of establishing tougher examinations, but did not take advantage of the offer to create an alternative position in this variation of the study. Extrapolating from their results, Maass and Volpato suggested that personal involvement may be necessary before creativity enhancement occurs in reaction to minority group influence. Such involvement is especially likely if the minority group members are in some way related to the majority group to which the subject belongs. That is, they are deviants from the majority, but otherwise entitled to membership in it. Further research remains to be done on this aspect of minority influence, but it strikes me as an interesting new road to follow. Given Maass's impressive record of productive research, it seems a good bet that results bearing on this issue will soon appear in the experimental literature.

### Resistance to the Minority: Psychologization and Vested Interest

Up to this point, the effect of the minority has been shown to be subtle and strong, affecting attitudes and even fundamental perceptions. However, such influence seems to contradict our ordinary experience, in which minorities do not appear to wield such power on our thoughts and actions. Why the divergence? Two papers presented at the University of Padua address this question.

In the first, Melanie Trost, Douglas Kenrick (Arizona State University), and Anne Maass (University of Padua) conducted a standard attitude change experiment. Undergraduate subjects were led to believe that a majority or minority influence source was advocating the institution of senior comprehensive examinations at their university. The personal relevance of this suggestion was manipulated by the suggested timeframe of the introduction: in the high relevance condition, the examinations

were to be implemented in the coming year; in the low relevance condition, a developmental period of 10 years was suggested.

In the low relevance condition, the standard minority group influence effect was found. Subjects were more favorable toward the examination suggestion when it was made by a minority source. However, under conditions of high relevance, the opposite was found. This result suggests that increasing the vested interest of an attitude decreases its relative susceptibility to minority influence (cf. Sivacek & Crano, 1982).

High relevance apparently transforms the phenomenon of minority conversion into something more aptly described as minority rejection, and it does so by altering the types of thoughts produced by the recipients of influence. Moscovici's formulation has viewed targets as harboring latent positive reactions to minorities. Trost's findings are perfectly consistent with this viewpoint in the low relevance context. However, the findings under high relevance indicate that the minority's advantage is a tenuous one. Under high relevance conditions, differential reactions to minorities and majorities are more reminiscent of findings on hostility toward outgroups.

Research by Stamos Papastamou, Panteios Faculty of Political Science, Athens, Greece, complements the observations of Trost and her associates. In his study, Papastamou was concerned with the process he has termed "psychologization." This process entails a misidentification of the motives or logic of a person who holds a position at variance from one's own. Basically, psychologization is the establishment of an apparent causal link between a person's position and his minority or majority status. In other words, psychologization is a means of rationalizing an opposing viewpoint: "He believes that because he is a member of Group X, and they all think that way."

In his inventive experiment, Papastamou undertook a minority influence attitude change experiment, but varied the conditions under which psychologization would, or would not, be expected to occur. Consistent with his hypotheses, he found that psychologization strongly attenuated minority group influence; however, it had little impact when a representative of the majority was the influence source. The fact that a majority member believed as he did because he was a member of the majority did not diminish his persuasiveness. However, such attenuation of persuasive impact was exactly the result when the influence source was a minority group member. Clues as to the reasons for this divergence of effects of psychologization as a consequence of minority or majority group influence can be found in the research of Robin Martin, Sheffield University, U.K., which follows in the next section of this report.

## Social Identification and Influence

Robin Martin's theoretical paper is useful in helping us come to grips with the phenomenon minority group influence, and in tying together the various strands of influence research to form a coherent cloth. Martin speculated about the nature of minority influence. In his view, minority positions are highly distinctive and visible. Accordingly, we try to explain a minority's views and often seek additional information. In other words, minorities encourage us to understand them. We usually (but not always) assume that people with minority views have negative characteristics; i.e., they are undesirable. Thus, if we agree with the minority view, we are seen by others as similar to this group and share its undesirable characteristics. As such, there is a natural resistance to being influenced by a minority. However, given the distinctiveness of the minority position, we often are sufficiently intrigued to work on understanding their position. This process of investigation and information search sometimes results in our being persuaded, either by the cogency of the arguments we have uncovered, or because we need to rationalize the efforts we have expended in confronting the minority position.

Martin's paper is relevant for Nemeth's and Maass's work, because it provides a rationale for understanding the power of the minority to induce divergent thinking or creativity. Minority positions are distinctive and do draw our attention. In the process of attending to such distinctive positions, we can develop creative or divergent responses. Martin also suggests a basis for understanding resistance to minority influence and acquiescing to majority views. In the case of majority influence, people are resistant in order to protect their valued beliefs, but they also find identification with the majority as reinforcing or beneficial. The resistance in order to protect cherished beliefs effect also holds true in the case of minority influence, but we also resist being identified with such sources. As such, the minority is put at an added disadvantage. However, since its message is distinctive and stimulates additional cognitive work, the disadvantage is not as great as it might be unless the context is such that the minority-inspired message can be rejected out of hand, as might happen in situations of high vested interest (cf. Trost et al., cited earlier). In such circumstances, the minority would be particularly disadvantaged, since its information would lose its advantage of distinctiveness while retaining its stigmatized outgroup status (and thus, not stimulate further investigation of its position). Research by Trost and by Papastamou is fully consistent with Martin's orientation.

I presented another context for understanding the variable influence of minority and majority influence sources. Reflecting on some recent research, I found that the subjectivity or objectivity of the decision-making task

had a major influence on people's susceptibility to ingroup (majority) or outgroup (minority) influence. In an earlier study, Gorenflo and Crano (in press) found that when people thought they were making a subjective judgment, they were very susceptible to majority group influence, but very resistant to minority influence. Under circumstances that involve a subjective belief, the observations of an outgroup are irrelevant, at best, and, are rejected. However, the ingroup position is quite relevant, and hence influential. In situations involving a statement of fact or an objective decision, the minority group position can be quite useful. Agreement with an obvious outgroup can signal the validity of one's position even more strongly than ingroup agreement can since the outgroup presumably does not share the same cognitive and perceptual biases as the ingroup; hence, their agreement would carry greater weight.

These results suggest that circumstances that promote the perception of a decision as subjective will severely weaken the influence of minority groups. When the situation is set up in such a way that the decision appears objective, then the minority can be expected to have a very powerful effect. I hope that when the fourth conference on minority influence is held, the ONREUR Liaison Scientist who attends will be able to discuss the outcome of studies that put these ideas to the test.

## References

Asch, S., "Effects of Group Pressure Upon the Modification of Judgment," *Groups, Leadership, and Men*, H. Guetzkow (Ed.) (Pittsburgh Carnegie Press, 1951).

Clark, R.D. III, & Maass, A., "Social Categorization in Minority Influence: The Case of Homosexuality," *European Journal of Social Psychology*, 18 (1988), 347-365.

Crano, W.D., "Effects of Sex, Response Order, and Expertise in Conformity: A Dispositional Approach," *Sociometry*, 33 (1970), 239-252.

Crano, W.D., *Conformity Behavior: A Social Psychological Analysis*, (Irwin, Homewood, IL.) Also included as Chapter 17 in *Psychology: A Programmed Modular Approach*, C.N. Cofer & H.E. Fitzgerald (Eds.), (Irwin, Homewood, IL, 1975).

Crano, W.D., *Conformidade de Comportamento: uma analise psicosocial* (tran. R. dos Santos). (Sao Paulo, Brazil, Ed. Brasiliense, 1978.)

Crano, W.D., & Messe, L.A., *Social Psychology: Themes and Principles of Interpersonal Behavior*, (Dorsey Press, Homewood, IL, 1982).

Festinger, L., "A Theory of Social Comparison Processes," *Human Relations*, 7, (1954), 117-140.

Gorenflo, D.W., & Crano, W.D. (in press), "Judgmental Objectivity-Subjectivity and Locus of Choice in Social Comparison," *Journal of Personality and Social Psychology*.

Maass, A., & Clark, R.D., III, "Internalization vs. Compliance: Differential Processes Underlying Minority Influence and Conformity," *European Journal of Social Psychology*, 13, (1983), 197-215.

Maass, A., & Clark, R.D., III, "The Hidden Impact of Minorities: Fifteen Years of Minority Influence Research," *Psychological Bulletin*, 95, (1984), 428-450.

Maass, A., & Clark, R.D., III, "Conversion Theory and Simultaneous Majority-Minority Influence: Can Reactance Offer an Alternative Explanation?" *European Journal of Social Psychology*, 16, (1986), 305-309.

Maass, A., Clark, R.D., III, & Haberkorn, "The Effects of Differential Ascribed Category Membership and Norms on Minority Influence," *European Journal of Social Psychology*, 12, (1982), 89-104.

Moscovici, S., *Social Influence and Social Change*, (Academic Press, London) (1976).

Moscovici, S., "Toward a Theory of Conversion Behavior." In L. Berkowitz (Ed.), *Advances in Experimental Social Psychology*, Vol. 13, pp. 209-239, (Academic Press, New York, 1980).

Moscovici, S., & Mugny, G. (Eds.), *Psychologie de la Conversion*, Cousset (Fribourg, CH, Delval, 1987).

Mugny, G., & Perez, J.A., *Le deni et al raison: Psychologie de l'impact Social des Minorites*. Cousset (Fribourg, CH, Delval, 1986).

Nemeth, C.J., & Kwan, J., "Originality of Word Associations as a Function of Majority vs. Minority Influence," *Social Science Quarterly*, 48, (1985), 277-282.

Nemeth, C.J., & Kwan, J., "Minority Influence, Divergent Thinking, and Detection of Correct Solutions," *Journal of Applied Social Psychology*, 17, (1986) 120-133.

Nemeth, C.J., & Wachtler, J., "Consistency and Modification of Judgment," *Journal of Experimental Social Psychology*, 9, (1973), 65-79.

Nemeth, C.J., Wachtler, J., & Endicott, J., "Increasing the Size of the Minority: Some Gains and Some Losses," *European Journal of Social Psychology*, 7, (1987), 15-27.

Personnaz, B., "A Study in Social Influence Using the Spectrometer Method," *European Journal of Social Psychology*, 11, (1981), 431-438.

Sherif, M., "The Psychology of Social Norms," (Harper & Row, New York, 1936).

Sivacek, J., & Crano, W. D., "Vested Interest as a Moderator of Attitude-Behavior Consistency," *Journal of Personality and Social Psychology*, 43, (1982), 210-221.

## SOLID-STATE PHYSICS

### Condensed-Matter Research at the École Polytechnique

by Dean L. Mitchell, the Liaison Scientist for Solid-State Physics in Europe and the Middle East for the Office of Naval Research European Office.

The École Polytechnique (EP) was instituted in 1794, during the revolutionary period (on the recommendation of Gaspard Monge and Lazare Carnot) to train scientists and engineers for government service under the Republic. It has served this role well and is considered today the premier institution in France for the training of engineers and scientists for military service, for governmental service, and for leading positions in industry. It is very much an elitist institution in a country that traditionally has been run by the elite.

The EP is run by the Ministry of Defense and is headed by an active service army general. However, the military associations are more a reflection of tradition than reality. The composition of the student body, the curriculum, and the flavor of the campus are more reminiscent of MIT than of West Point.

The EP moved to its present campus, a park-like setting near Palaiseau, about 10 years ago. Previously, it was located in Paris near the École Normale Supérieure and

near the University of Paris research center at Place Jussieu. The EP is somewhat more remote in its present location, 20km south of Paris. However, there is a concentration of other research centers with related research interests at Orsay, which is only a few kilometers away.

Physics research at the EP is carried out in eleven laboratories or research centers that are located in the Physics Department. Five centers concentrate on solid-state and condensed-matter physics or on related topics in optics.

My visit was limited to the Laboratoire de Physique de la Matière Condensée (PHMC), which is one of several laboratories at the EP that is supported by the Centre National de la Recherche Scientifique (CNRS). Professor I. Solomon, former laboratory director, has been replaced by B. Sapoval but continues as the group's research mentor and is active in the conduct of his own research.

Research projects in the PHMC laboratory are grouped in five general topical areas. The main research topics and senior research investigators of each are

- Fractals-B. Sapoval, M. Rosso, and J.F. Gouyet
- Semiconductor/Electrolyte Interface-J.N. Chazalviel
- Photoemission-G. Lampel
- Sol Gels-J.P. Bailot
- 1-D Nuclear Magnetic Resonance-F. Devreux

In addition to the senior research investigators, there is an equal number of younger researchers supported by the CNRS or defense ministry. Including graduate students and technicians, there is a total of about 50 laboratory personnel.

The photoemission group, headed by G. Lampel, has had remarkable success in adapting an old technique--cesiated cathodes--to the development of new photo-electron spectroscopies for the investigation of the electronic levels and extended band structures of semiconductors. It has long been known that a surface layer of cesium applied to metals used in cathodes for photo-diodes and photo-multipliers lowers the work function for escape of electrons from the metal into the vacuum. It also has been well known that cesium on the surface of certain semiconductors can reduce the work function and even induce a negative affinity for electrons; i.e., the electrons are free to escape into the vacuum.

Lampel used these effects to develop new photo-emission spectroscopies which are employed to investigate the band structure and surface states in semiconductors. First, selectively tuned radiation is used to excite electrons into higher-lying conduction states. With cesiated surfaces, the excited electrons are then free to escape into the vacuum where their number and energy distribution may be measured. Spin-dependent phenomena may be studied by using circularly polarized radiation for excitation. Lampel and his group also have successfully carried out the inverse experiment--injecting electrons from the vacuum into higher-lying states in the semiconductor with observation of the subsequent decay by photo luminescence. A description of a spectrometer to measure the energy distribution and the spin polarization of electrons in semiconductors is provided in the Review of Scientific Instruments, 57, 1052 (1986).

Using such techniques, the photoemission group has developed a spin-polarized electron source with quantum yields of a few percent and polarization efficiencies of 30 percent at 300K or 36 percent at 120K. The sources were fabricated by placing a 100 Angstrom cap of gallium arsenide (GaAs) on top of aluminum gallium arsenide (Al-GaAs). The alloy composition was selected to match the band-gap for excitation with the photon energy of the helium neon laser.

These techniques have been applied successfully to measure band-edge features in silicon, in AlGaAs hetero-

lattices, in AlGaAs alloys, and in AlGaAs quantum well structures. Research is now underway to extend the application of these techniques by using external electric fields to enhance the photoemission.

The research group within the PHMC, headed by B. Sapoval, is studying the fractal nature of interfaces for various physical processes such as diffusion, invasion, and corrosion. The approach is mainly by using computer simulations to both test and aid in the formulation of theoretical concepts and analytical relations. These studies have roots in the extensive studies of percolation and localization/delocalization phenomena that have been carried out over the last two decades to better understand disorder phenomena. However, the focus since about 1985 has been to develop a more physical basis for understanding the interfacial processes and configurations by applying the insights that have been developed for treating fractal geometries.

Some of these successes include the description of binary interdiffusion. This is an analogous problem to that of percolation in a concentration gradient. In the case of binary diffusion on a square lattice, the interface cannot be described in terms of a single diffusion front but rather requires two fronts. The complex object representing the diffusion front was shown to have fractal properties with a fractal dimensionality of 7/4.

The evolution of the diffusion front, as revealed by computer simulations, exhibits instabilities in which sections of the front undergo macroscopic changes over a very short period. The periods of rapid change are followed by long periods of stability. The noise spectrum of these fluctuations includes frequency components that are very high compared with the hopping rate for single atoms. This fractal noise has been calculated by Monte Carlo simulations for the two-dimensional case. Using scaling arguments inferred from the simulations, they predict a high-frequency power noise spectrum with a variation as  $1/f^2$  and a low-frequency variation as  $1/f$ . The crossover is predicted to occur at a frequency that is determined by the gradient at the interface.

Professor Solomon remains the scientific mentor for the group even though he is no longer active in laboratory management. His own research in recent years has concentrated on studies of amorphous silicon. When the amorphous semiconductor craze began in the early 1970s, Professor Solomon assumed the role of coordinator for research on amorphous semiconductors in France. Under his general coordination, the participating laboratories were able to concentrate their research efforts in a cooperative rather than competitive manner. The early program of informal interactions later grew into a large national program supported by the CNRS with Solomon continuing as coordinator in a more formal role.

The CNRS-supported program of basic research ultimately led to commercial development of solar cells in

France using amorphous silicon. Professor Solomon participated directly in this development and was associated for many years with the company that brought the cells into production. The small French development company that nurtured this commercialization has recently been absorbed by a large automobile oil company conglomerate. A possible market is seen for cheap solar cells as standby power supplies for airconditioning cars left in the sun. Solar cells are advantageous since the maximum power demand occurs at the same time that the cells receive the maximum light flux.

More recently, Solomon has been part of a collaborative effort with scientists at the Center National d'Études des Télécommunications laboratory in Bagueux to develop thin-film, electro-luminescent (EL) memory displays that have improved contrast ratios over present displays. The key feature of this panel display is the inclusion of a thin photo-conductive (PC) layer of amorphous silicon in the sandwich structure of the display panel. Thus, the impedance of the PC layer is high in the *off* state with most of the applied voltage appearing across the silicon layer. However, after switching, the silicon layer is low impedance so that the voltage drop is mainly

across the active EL layer. The process is hysteretic, so that the display has inherent memory.

The intrinsic contrast of the panels is 3,000 compared with 100 for conventional EL displays. The maximum *off* luminance is 0.2 cd/sq.m at 1kHz. This is smaller than standard EL displays by more than one order of magnitude. Working displays have been fabricated by France Telecom but there does not appear to be any interest in commercialization.

Overall, condensed-matter research at the EP appears quite healthy. There is a good mix of basic research on topics of fundamental and long-range interest; e.g., fractals, as well as research on topics with potential contributions to technology in the shorter term; e.g., displays and spin-polarized cathodes. This mix appears to be in line with the new directions for research that the CNRS is encouraging. My sense was that the laboratory is presently quite well supported but is not as well equipped as equivalent laboratories in Germany. This deficiency is offset by the high quality of the students who continue to be attracted by EP's elitist status among educational institutions in France.

## NEWS, NOTES, AND ABSTRACTS

### Errata

In ESNIB issue No. 89-07, News and Notes article "Dutch Marine Information Service," should have been credited to CDR John P. Simpson.

### Meeting Announcement

Mr. Gerald S. Malecki

Topic: 10th European Meeting on Cybernetics and Systems Research  
 Dates: April 17-20, 1990  
 Sponsor: Austrian Society For Cybernetic Studies In Cooperation With University of Vienna  
 Department of Medical Cybernetics and Artificial Intelligence  
 Location: University of Vienna, Austria  
 Chairman: Robert Trappi, University of Vienna

Plenary lectures and symposia on  
 • General Systems Methodology

- Fuzzy Sets and Systems
- Cybernetics in Biology and Medicine
- Cybernetics of Socio-Economic Systems
- The Management and Cybernetics of Organizations
- Innovation Systems in Business and Administration
- Robotics and Flexible Manufacturing
- Systems Engineering and Artificial Intelligence for Peace Research
- Communication and Computers
- Artificial Intelligence
- Parallel Distributed Processing in Man and Machine.

The call for papers and other meeting information are available from:

Secretariat, EMCSR 90  
 Tenth European Meeting on Cybernetics and Systems Research  
 Austrian Society for Cybernetic Studies  
 Schottengasse 3  
 A-1010 Vienna 1  
 Austria  
 TEL: 43 222 535 32810  
 FAX: 43 222 630 652  
 E Mail: sec@ai-vie.uucp

## Book on Psychology and Torture to be Released

Dr. William D. Crano, currently on leave of absence from Texas A&M University, is serving as the Director of the Program in Social Psychology at the National Science Foundation, Washington, D.C.

Richard Snow, former ONR Liaison Scientist in Psychology, described some interesting observations on the psychology of torture (ESNIB 85-09:406). He was reporting on a recent visit to Greece, and had talked with several people whose lives had been touched by the torture of political prisoners in Greece. This is a fascinating topic, about a practice that is all too common in the world's societies. *Psychology and Torture* edited by Dr. Peter Suedfeld, will be released by Hemisphere Publishing Company, Washington, D.C.

## Resonance Vibration Can Cause Engine Failure

Dr. David Feit

A June 14, 1989, report in the London Times suggests that the recent crash of a British Midlands Boeing 737-400 passenger jet may have been indirectly caused by an engine failure attributed to a vibration resonance phenomenon. In early June, a similar problem was encountered on two identical airliners, which led to the grounding of all British-registered 737-400 series planes.

Investigators now believe that a resonance frequency of the fan blades occurs within the operating range of the engines. Such a condition can lead to a fatigue failure (breakup of an object caused by a large enough stress repeated over many cycles) of the blades ultimately causing the destruction of the engine. In the case of the British Midlands crash, one of the engines failed because of the resonance phenomenon, but the crew mistakenly shut down the remaining good engine.

The CFM 56-C3 engine is produced by CFM International, a consortium formed by Societe National d'Etude et Construction de Moteurs d'Aviation (SNECMA), a French engine manufacturer, and General Electric of the United States. When Boeing introduced the 737 400-series, it required engines with larger thrust to carry more passengers over larger distances. To meet this requirement, CFM engineers redesigned the engines to create 1,500 pounds of additional thrust, which was achieved by a 4-percent increase in rotation speed and modifying the blade leading edge design. This engine, like others, has a cowling that is flat on the bottom to minimize the possibility of engine scraping along the runway on takeoff.

This combination of factors is now believed to have caused the unusual resonance condition leading to the engine failures. Despite the many hours of testing that an

engine must undergo before certification for commercial use, the peculiar condition of a steep climb with a full load at maximum power may not have been encountered earlier.

The engine manufacturers have advised operators outside the U.K. who are still using the engine to reduce power on takeoff to 90 percent of maximum. If further testing corroborates the theory of resonance vibration in the CFM 56-C3 engines, airlines would most likely replace these engines on existing aircraft with the earlier CFM 56-3B design, which is widely used on the Airbus A320 and Boeing 737-300.

## Gesellschaft für Mathematik und Datenverarbeitung mbH, Sankt Augustin, Federal Republic of Germany

Dr. Richard Franke

The German National Research Center for Computer Science (GMD) was founded in 1968, with its headquarters in Schloss Birlinghoven, a beautiful turn-of-the-century castle housing a significant collection of 16-18th century painting from the Italian and Dutch schools. The GMD presently has an annual budget of nearly DM 150 million (about \$75 million). About 75 percent is provided by the German government (Federal Minister for Research and Technology), the state of North Rhine-Westphalia (Minister for Science and Research), and the state of Hesse (Minister for Science and Arts), with the rest coming from contracts. The GMD employs about 1,300 persons (900 scientists) at the headquarters in St. Augustin, at Bonn and Darmstadt, and in research centers at the Technical University of Berlin, the University of Karlsruhe, and the University of Cologne. Liaison offices in Washington, D.C., Berkeley, California, and Tokyo, Japan, coordinate international cooperation. Research activities are primarily related to information technology and its promotion for the future.

The research and development activities of GMD are focused in ten long range scientific projects:

- Massive parallel systems
- Scientific supercomputing
- Knowledge-based design of integrated circuits
- Innovative programing and computer systems
- Software factory
- Integrated communication systems and services
- Open and distributed broad band systems
- Assistance computer
- The thinking book
- Supercomputer center.

The GMD expects to be able to pursue long-term goals, little affected by short-term economic constraints, and to play a neutral role among science, industry, and

users. Through consultation, they try to bring together expectations of the users and the reality of scientific and manufacturing capability. In addition, they promote technology transfer in the public interest and initiate new production processes.

Several of the projects are related to the SUPRENUM parallel supercomputer project, probably the best known activity of the GMD.

## A Conversation with Robert Dautray at the Headquarters of the French Atomic Energy Commission in Paris

Dr. Marco S. Di Capua

Robert Dautray directs the Inertial Confinement Fusion Branch of the Division of Military Applications of the French Atomic Energy Commission (CEA-DAM) (ESNIB 89-07:74). Dautray represents the best of the science technocrats educated in the French "great schools" (Barsoux, 1989) system. These schools, dating from the Revolutionary era, have bred a class of dedicated French engineer/civil servants endowed with three outstanding qualities--vision, agility, and persistence. Vision is their key to the course of the future, agility allows them to select optimal courses under changing political winds, and persistence sustains their momentum in politically foul weather (common in a multiparty democracy).

These admirable qualities, in scientist administrators like Dautray, I believe, have been one of the keys to French technological and economic progress. This progress also relies on a foundation of careful planning and public investment on key technologies. Obvious examples of this process are the Paris rapid transit, the national railways, the telephone network, the nuclear electricity program, and strategic weapons programs.

Born in 1928, Dautray is an alumnus of one of the "great schools"--École Polytechnique--created by the 1794 convention at the instigation of the mathematician Gaspard Monge and the engineer Lazare Carnot to: "...form engineers in all branches, re-establish the teaching of exact sciences and to provide a high scientific formation for young people both to be employed by the Government in the works of the Republic and to teach and pass on useful knowledge."

As Scientific Director of CEA-DAM, Dautray has served France with distinction. As a scientist, leader, and administrator, he has been involved in the French nuclear weapons program from its inception. Dautray has also played a key role with Karl-Heinz Beckurts, Nuclear Research Center, Karlsruhe, Federal Republic of Germany, in the design and construction of the research reactor facility of the Institut Laue Langevin, Grenoble, France. In addition to his scientific leadership, Dautray and his co-

workers, coauthored a reference textbook on mathematical analysis and numerical methods for science and technology (Dautray 1985, 1988, 1989). In 1977, Dautray was inducted into the mechanical sciences section of the French Academy of Sciences and holds the decoration as Commander in the Order of the Legion of Honor. Recently, Dautray was elected president of the scientific steering committee of the French National Center for Space Studies (CNES).

Dautray first discussed his vision of inertial confinement fusion (ICF) suggesting that an ICF laser driver that delivers 10 MJ of light at 0.3 microns is beyond the reach of even rich countries such as the U.S., Japan, or France. And even if the budgets were available, there is not yet a clear choice between a solid state laser (glass) and excimer laser. Therefore, Dautray believes that cooperation through a binational agreement holds the key to progress in ICF.

An obvious question that arises is why binational and not multinational. Dautray cited his experience with the French/German collaboration in the Laue-Langevin research reactor program as an example of successful implementation of binational scientific programs. Implementation of a program involving more than two countries could be difficult when the program may be intimately connected with issues of national and international security. Therefore, Dautray feels it is far better for two countries to establish the ground rules, as in the case of the Laue-Langevin collaboration, and allow others to join the operational project later.

Such a binational agreement could begin with a choice of laser technology milestones and scientific goals for a joint research program. Cooperative parallel development programs could follow. These mutually agreed-upon choices and development programs could lead to a commitment to build an ICF laser driver. The understanding developed between the scientific teams of the two countries would have to build confidence in the scientific, technological, and administrative skills of both countries so that more complete scientific results could be shared on a balanced give-and-take basis.

Dautray views the above proposition as a simple experiment in social science that would test the maturity of both nations at scientific, administrative, and political levels. The fundamental issue, of course, is building up sufficient trust and commitment to assure the success of the program in times of uncertainty and crisis. Dautray has proven to be quite adept at shepherding such programs in spite of the shifting winds of French politics.

Dautray feels that a background for such agreements already exists, and cited the agreement to build the Phoebus glass laser at Limeil and collaborative experiments on the laboratory X-ray laser program as fruitful examples of this approach.

Dautray also believes that even though magnetic confinement fusion may be close to scientific breakeven, there are sufficient nonlinearities that extrapolation of the scientific breakeven to economic breakeven may not be possible. Dautray believes that Inertial Confinement Fusion, notwithstanding uncertainties in the laser driver, may stand a better chance of being the winner in the long term.

A second area where binational agreements would be fruitful, according to Dautray, is a survey of the radiative balance of Earth from space orbit. He believes that national laboratories and the space agencies of the two countries have enough experience to field instrumentation to survey land masses, oceans, and the biosphere for radiation inputs and outputs, energy transport thorough the water cycle including surveys, with space-borne radars, of the water content of the first 50 or so meters of Earth's crust. This research area coincides with some of the objectives of NASA's Earth Observing Satellite mission proposed by a study group led by Sally Ride in 1987. In this mission, a satellite system would correlate, in an unprecedented way, detector data from many sensors to understand the interaction of Earth, water, and sky.

### Summary

Robert Dautray is a legendary figure in French scientific circles. He is a well-respected, first-class scientific leader, with a finely honed sensitivity to important unsolved problems; a very patient, well-connected, agile, and astute politician; and a very able administrator. The combination of these qualities will guarantee that his voice will be heard in CEA and space research scientific circles for many years.

Dautray's views and proposals reflect the maturity and confidence of contemporary French science and suggest that France enters the last decade of the 20th century in a scientific research leadership position.

### References

Barsoux, J. L., "Engineering Education in France: Leaders for Every Occasion," *IEEE News*, January 1989, reproduced in *Optoelectronics Reports*, 67 (1989); also: Lawrence P., and J. L. Barsoux, "Management in France: Quality and Exclusion," Cassell, London (1989).

Dautray, R. and L. Lions, *Analyse Mathématique et Calcul Numérique pour les Sciences et les Techniques*, Masson, Paris, Volumes I (1984), II, and III (1985).

Dautray, R. and L. Lions, *Analyse Mathématique et Calcul Numérique pour les Sciences et les Techniques*, in nine volumes: 1. *Modèles Physiques*; 2. *L'Opérateur de Laplace*; 3. *Transformations, Sobolev, Opérateurs*; 4. *Méthodes Variationnelles*; 5. *Spectre des Opérateurs*; 6. *Méthodes Intégrales et Numériques*; 7. *Évolution: Fourier*

*Laplace*; 8. *Évolution: Semi-groupe, Variationnel*; 9. *Évolution: Numérique, Transport* (1988), Masson, 120 Boulevard St. Germain, Paris 75280 Cedex 06.

## The European High Performance Laser Facility, Laboratory for Utilization of Intense Lasers, École Polytechnique

Dr. Marco Di Capua

At the beginning of 1989, French National Scientific Research Council (CNRS), British Science and Engineering Research Council (SERC), the Spanish Higher Council for Scientific Research (CSIC) (ESNIB 88-01:61-62), the Italian Atomic Energy Council (ENEA), and the Max Planck Gessellschaft, Federal Republic of Germany (FRG), tasked a committee to explore European interest in a blue or near UV 100-kJ laser facility that would be operational within 5 years of the signing of an agreement. This facility would produce high-energy density in matter allowing participating members to perform research on: laser beam-plasma interactions, physics of high-energy density matter including topics in fundamental atomic physics and spectroscopy, X-ray lasers, noncoherent X-ray sources, astrophysical plasmas, X-ray laser applications to chemistry and biology, and the production of energetic pulses of particles such as neutrons or alphas.

The committee is convened by three experienced physicists in the field: Edouard Fabre, director of the LULI Laboratory in France; Michael Key who heads CLF at RAL; and Frederick Schaeffer, director of the IBC Max Planck Institute, Goettingen. In addition, the committee includes representatives from France, FRG, Great Britain, Italy, and Spain. Deliberations are converging on a scientific program, the rationale for the choice of a glass or excimer laser, and the nature of the experimental facility. The proposal should be completed in January 1990.

The European High Performance Laser Facility proposal responds to the need for a civilian European research facility that, extending beyond national facilities available in Europe, is competitive with open facilities in Japan and the U.S. This facility would be a logical European extension for national science laboratories such as CNRS--Laboratory for Utilization of Intense Lasers (LULI) Laboratory at École Polytechnique; SERC; nationwide Central Laser Facility (CLF), Rutherford Appleton Laboratory (RAL), U.K.; or the ASTERIX IV facility, Max Planck Institut for Quantenoptik in Garching, FRG.

The 100-kJ laser would leap 1 1/2 orders of magnitude in energy from national civilian European facilities, adding a European dimension to research on the physics of high energy density. Present facilities are: VULCAN, at

CLF, RAL, a 1.053- $\mu\text{m}$  Nd-Glass laser that delivers a 1-ns / 2.4-TW / 2.4-kJ pulse (ESNIB 88-09:21-22, and EOARD-LR-88-21); the LULI facility, 1.053- $\mu\text{m}$ , 0.6-ns / 1.2-TW / 1-kJ pulse; and ASTERIX IV at MPQ, a 1.315- $\mu\text{m}$ , 2-ns / 5 -TW / 3-kJ iodine laser (ESNIB 88-03:64-66, and EOARD-LR-88-50). As user-oriented facilities, VULCAN and LULI support many experiments from other institutions as well as in-house programs. ASTERIX IV is dedicated to MPQ research.

As a comparison, the Lawrence Livermore National Laboratories (LLNL), University of California, recently produced 125 kJ of 1.053  $\mu$  light exceeding its 120-kJ performance specification (Coleman, 1989).

The commitment would be to develop a facility where the common research thread is the physics of matter at high energy densities and other fundamental studies in the interaction of intense laser beams with matter. Even though at present it may not be possible to explore all the physics the facility is capable of, the committee feels that there is sufficient fundamental research to justify constructing a highly needed European open facility to serve the widest possible international constituency.

#### References

Coleman, L., "New Fusion (sic) Energy Record by Lab's Nova Laser," *Newline* (LLNL), Vol 14, No. 14 (1989), 1.

### International Symposium on Advances in Corrosion Protection by Organic Coatings; and University of Trondheim, Norway, and University of Manchester Institute of Science and Technology, U.K.

Dr. Martin W. Kendig, Rockwell International Science Center, Thousand Oaks, California

#### Introduction

In April 1989, I presented two papers at the Cambridge Symposium on Advances in Corrosion Protection by Organic Coatings. One paper described work done under Office of the Chief of Naval Research (ONR) contract, "Environmental Integrity of the Coating/Metal Interface." D. Scantlebury, University of Manchester, Institute of Science and Technology (UMIST), and I organized the symposium. While overseas, I also visited the Foundation for Science and Industrial Research at the Norwegian Institute (SINTEF) group, as well as the Electrochemistry Group at the Norwegian Technical Institute (Norges Tekniske Høgskole [NTH]), and the corrosion group at UMIST. I evaluated the directions and levels of effort by these institutions in corrosion and corrosion protective coatings.

### The Cambridge International Symposium on Advances in Corrosion Protection by Organic Coatings

In organizing this meeting, Scantlebury's and my objective was to present a forum for the most recent advances in characterizing the fundamentals of corrosion protection by organic coatings and improving the corrosion protection provided by organic coatings. Forty-six talks were presented to approximately 125 delegates at the 4-day meeting. The talks were divided into four categories: (1) adhesion, disbonding, and underfilm corrosion; (2) novel polymers and application methods; (3) electrochemical techniques and interpretation; and (4) pigments and additives for corrosion performance. More papers fell into categories 1 and 3 which reflects the general ease of measuring and categorizing failures rather than suggesting solutions. By making this observation, I do not mean to minimize the importance of knowing corrosion mechanisms in great detail, but wish to point out the need for applying some of this knowledge.

A copy of the extended abstracts has been forwarded to J. Sedriks of ONR and the titles of presented papers may be obtained from me at 1049 Camino dos Rios, Thousand Oaks, California 91360. For the most part, the papers represented fresh approaches to the problems of corrosion protection by organic coatings.

**Adhesion.** J.E.O. Mayne, University of Cambridge, the "dean" of corrosion protective organic coatings research, gave an interesting and relevant paper on the nature of nonsolvent coatings. Using his resistance method of characterizing organic coatings, he demonstrated that a nonsolvent epoxy showed superior barrier properties compared to solvent cast films. However, the nonsolvent epoxy had inferior adhesion which could be improved temporarily with organo-silane adhesion promoters or the plasticiser dibutyl phthalate.

van Ooij, Colorado School of Mines, Golden, continued the theme of environmentally benign coating systems. van Ooij described a nonchromate treatment to stabilize phosphate conversion coatings. The treatment entails rinsing in a silicate solution followed by treatment with an organo silane. Leidheiser, Lehigh University, Bethlehem, Pennsylvania, also proposed a post-treatment for phosphated steel by electrodeposition of a partial layer of Zn in regions not covered by phosphate crystals.

Perhaps a better solution to the complexities of adhesion-promoting conversion layers was suggested by Funke, University of Stuttgart, Federal Republic of Germany (FRG), who suggested that thin organic films ( $< 1\mu\text{m}$ ) should replace inorganic conversion coatings for adhesion. Since there is no reliable corrosion protection of metals without good wet adhesion, interfacial layers such as phosphate are typically used to promote adhesion. Funke suggests that highly crosslinked, high Tg (glass transition temperature) organic layers might provide the necessary wet adhesion. If they are thin enough,

they do not require the same elongation necessary for thick films. Funke's ideal picture of corrosion protective organic coatings includes several layers each of which has specific functions—a thin, high Tg adhesive layer, a barrier layer having low water and oxygen transport, a top layer of high gloss and good optical properties. R. Taylor, University of Virginia, presented data on ultra thin graded interfaces formed by energetic ions. It may be possible that electropolymer layers as described by us for Mg and Mengoli and Musiani, University of Padova, Italy, for steel could be used for adhesive interlayers.

The role of mechanical properties of the organic film at the interface during environmental exposure was considered to be very important. We presented an acoustical microscopic method that serves to characterize changes in the mechanical properties of the interface of thin organic films. Our results for a modified butadiene showed how surface energy changes and alkaline attack under cathodic conditions serve to degrade adhesion. J. Watts, University of Surrey, U.K., presented a few recent results on a similar system giving a now well-documented picture of the polybutadiene steel interface to consist of an interphase of Fe(II) oxides and carboxylate species.

**Electrochemical Methods.** Electrochemical methods for evaluating corrosion protective organic coatings are still dominated by electrochemical impedance as evidence by work presented by J. Titz, BASF Corporation, Ludwigshafen, FRG; F. Mansfeld, University of Southern California; K. Umeyama, Furukawa Research Electric Co., Ltd., Kanagawa, Japan; W.W. Tait, S.C. Johnson & Son Inc., Racine, Wisconsin; D.J. Mills, Paint Research Association, Teddington, U.K.; and J.N. Sykes, Oxford University.

Mansfield and Umeyama both presented models for evaluating cathodic disbonding. Umeyama's model entailed a scribe. The logic behind his approach for extracting a figure of merit from the impedance spectrum was not entirely clear. Mansfeld essentially presented Haruyama's model with a new suggested parameter. The Haruyama model maintains that the parallel resistance of the coating results from disbonding. From my point of view, this is not consistent with previous results obtained for free films which, by design, are totally disbonded but show no decrease in resistance.

Sykes uses an electrochemical transient to evaluate closely spaced time constants associated with the coated surface, and maintains that the method allows better resolution of closely spaced time constants. Sykes may be right, although there remains some sampling problems with his method (low-frequency data are not measured with the same sensitivity as high-frequency data).

B. Skerry's, Sherwin-Williams, electrochemical noise analysis seems to, in effect, provide a measurement of

coating resistivity and, hence, correlates quite well with coating behavior.

Sadkowsky, Flis, et al., Polish Academy of Science, Warsaw, described an interesting application of an impedance approach using a low-frequency impedance method to follow the phosphatizing process. The method allowed determination of the time required to nucleate and precipitate the phosphate layer. Their analysis not only provided for an evaluation of the kinetics of phosphatizing, but also gave information on the integrity of the resulting phosphate layer. The results illustrated the effectiveness of an alkaline degreasing and activating in a titanium compound suspension. Although not specifically mentioned by the authors, this method could be useful for in-plant quality control of phosphate baths as well as being a research tool.

Regarding impedance methods, there was a near consensus at the meeting that coatings that exhibited early resistances above  $100 \text{ M ohm cm}^2$  will remain protective over extended exposures.

Sekine, University of Tokyo, presented a scanning vibrating probe method as a nondestructive, *in situ* way to evaluate the galvanic currents between a scribe and the coated surface. Although I did not understand the need for his elaborate statistics, the approach represents a unique method for evaluating these currents. Whether the method can be generalized to coatings thicker than 10  $\mu\text{m}$  and environments other than 30 percent aqueous acetic acid remains to be seen.

**Inhibitors/Pigments.** Several of the papers dealing with novel corrosion inhibitors/additives were motivated by environmental concerns. Braig, Ciba-Geigy, Switzerland, described an organic inhibitor as a possible replacement for chromate. Yamamoto, Nippon Paints, Japan, described a vanadate-phosphate; and Agarwala, Naval Air Development Command, Warminster, Pennsylvania, gave an update on the microencapsulated inhibitors under development by L. Bailin, Lockheed. None of these approaches appear to be really viable substitutes for chromate or truly environmentally benign at this time. They represent some progress in the right direction.

The interface between coatings and inhibitors was dealt with by Scantlebury who presented a paper on complexing agents as inhibitors/film formers. Scantlebury showed that the compounds inhibit by both complexing (in corrosive organic media) and noncomplexing (in NaCl solutions) modes.

W. Fischer, Markische Fachhochschule, Iserlohn, FRG, presented an unscheduled talk on life prediction of organic coatings. He integrated several predictive tests including impedance measurements, and open-circuit potential and other coating properties to predict coating life. Fischer's basic approach appeared to provide a good basis for a possible expert system although this was not brought up at the meeting.

**Meeting Summary.** Overall, the main interests of the international protective organic coating community appear to be directed toward making simpler, environmentally benign coatings that are more adherent under wet, corrosive conditions. Elimination of solvents, conversion coatings and harmful pigments represent important goals. Electrochemical evaluation of loss of adhesion and life prediction using electrochemical methods remain important areas of research. Disappointingly, few nonelectrochemical, *in situ* methods were described.

#### NTH-SINTEF

Georg Hagen (my contact at NTH) had previously collaborated with me at the Science Center several years ago on some photoelectrochemical studies of the passive films on aluminum (Al) and electrochemical noise. The primary focus of the corrosion-oriented staff of both the electrochemistry department and SINTEF remains development of Al processing (molten salt studies by J. Thonstad and R. Tunold) and improved corrosion resistance of Al and magnesium by elimination or counteraction of adverse effects of inclusions and intermetallics (K. Nisancioglu of NTH and H. Sigurdsson of SINTEF). There appears to be some effort to promote high purity Al for offshore structures. The search for a *stainless* Al is alive and well at Trondheim. Alloying constituents such as molybdenum, chromium, and cerium have been mentioned along with rapid solidification. No effort in the area of Al-Lithium alloys or metal matrix composites (MMC) was apparent.

G. Hagen and R. Odegard, electrochemists, described new thrusts in the area of applying conducting polymers for corrosion protection and sensors. Some collaboration exists between Odegard and Skotheim, Brookhaven National Laboratory (BNL), Long Island. G. Hagen and R. Odegard described a recent discovery that they made of an anodic polymerization of methyl thiophene to give a film which shows a cyclic voltammetric response sensitive and selective to nitrate ion. Some work on the application of polypyrrole for corrosion protection of stainless steels is being considered.

G. Hagen still pursues analysis of electrochemical noise for corrosion monitoring of Al. However, most of the results are theoretical based on exercising a Monte Carlo model that he and I developed several years ago. One problem with evaluation of electrochemical noise of Al is the extremely low frequencies required and, hence, long collection times.

Study of corrosion protective organic coatings is primarily performed by U. Steinsmo, SINTEF, who recently completed post-doctoral work at BNL directed by Hugh Isaacs. Steinsmo polarizes steel specimens coated with 100-300  $\mu\text{m}$  of paint from open circuit to -700 mV while measuring the current to obtain the film resistance. She sees no one-to-one relationship between this resist-

ance and ability of the coating to protect in long-term fresh water exposure, but considers the paint film resistance as one of several factors governing coating life. This work was also presented at the Cambridge meeting. Steinsmo described some preliminary concepts for experiments to determine whether cathodic disbonding is dominated by cation transport through the film or laterally from the defect using auger electron spectroscopy and cesium ion electrolytes.

#### UMIST

At UMIST, I talked with R. Cottis, S. Turgoose, R. Newman, and J.D. Scantlebury and discovered some interesting approaches to old problems.

R. Cottis outlined a proposed eddy current method for detecting early fatigue damage. The novelty of his approach lies in using the frequency dependence of the cell impedance to isolate different effects, perhaps to isolate fatigue damage from geometric effects. Cottis plans to use a Solartron frequency response analyzer rather than a network analyzer. Corrosion scientists have more experience with the former apparatus typically used for measuring the electrochemical impedance spectrum.

S. Turgoose continues an effort aimed at gaining a mechanistic understanding of the role of corrosion inhibitors and corrosion inhibiting pigments in paint films. Turgoose's approach relies heavily on modeling or reproducing the actual chemical environment in which the pigment acts. He has used coplanar electrodes (similar to Mansfeld's atmospheric corrosion monitors) to characterize under-film electrochemistry. Turgoose has also used precipitated inhibitors in filter paper to form model-free films of inhibitors such as products of Pb with azelaic acid.

I spoke briefly with R. Newman who has several active projects. Newman was most interested in a probabilistic model for the dissolution of an alloy. The model uses a cellular automata-type approach to predict dissolution or passivation. The model apparently predicts correctly the required percent of Cr in iron to form stainless steel. Currently, he is completing a detailed analysis of the results of this model. Newman is also working on an electrochemical approach to monitor the wear of composites and microbiological corrosion.

J.D. Scantlebury uses low volatile organic component (VOC) coatings (based on liquid epoxies such as Epikote 828) in his work although his main interest is developing a basic understanding of adhesion. Scantlebury claims to have developed a method based on fundamental fracture mechanics to determine the strain energy release rate from analysis of force transients resulting from falling weight impact. He mentioned a concept of chemical fatigue shown by films cyclically exposed to a given environment/solvent.

## ONREUR REPORTS AND MAS BULLETINS

### MAS Bulletins

The following Military Applications Summary (MAS) Bulletins were published between 27 July and 29 September 1989. The MAS Bulletin is an account of accomplishments in European naval research, development, and evaluation. Request copies by number from ONREUR.

42-89	Second Generation Crewserved and Individual Served Weaponsights
43-89	Aquamesh Fiber-Optic Alarmed Underwater Security Barrier
44-89	MW 08 Multi-Beam Air and Surface Surveillance Radar
45-89	High Performance Electro-Luminescent Memory Display
46-89	Strip Laminate Rocket Motor Cases
47-89	NATO Establishes Insensitive Munitions Information Center

## REPORTS ON EUROPEAN SCIENCE AND TECHNOLOGY FROM OTHER COMMANDS

### Reports

Information on each of the reports listed below was furnished by the following activity. Address requests to:

**EOARD** - European Office of Aerospace Research and Development, Box 14, FPO New York 09510

#### Chemistry

*Chemistry and Materials Science Research in Turkey*, by LTC Chet Dymek, EOARD. (16pp) [EOARD-LR-89-051]

Two research institutions in Turkey are conducting research in materials science and related chemistry. The Middle East Technical University (METU) in Ankara and the Marmara Scientific and Industrial Research Institute (TUBITAK) in Gebze are developing R&D programs designed to provide the technology base for Turkey's very young technology industry. A promising research program at these institutions has been proposed on the combination of mechanical alloying with oxide dispersion strengthening of the Ti-Al and Ni-Al intermetallics. A strong program in synthesis and characterization of phthalocyanines with crown ether moieties may also be of potential interest.

*Technical University of Denmark: Electrochemistry and Surface Chemistry*, by LTC Chet Dymek, EOARD. (15 pp) [EOARD-LR-89-053]

In 1973, the Technical University of Denmark was moved from Copenhagen to its present location at Lyngby. Since that time, they have maintained very strong pro-

grams in electrochemistry and surface science. Professor Bjerrum's group is involved in several projects; e.g., relatively low-melting salts, including battery concepts, refractory metal deposition, Raman spectroscopy of species in melts, and precision measurements of salt properties at high temperatures and pressures. Professor Birdi's group is engaged in high-precision techniques for measurement and interpretation of surface phenomena. Dr. Begtrup's group is developing new techniques for the synthesis of azoles with substituents that make them difficult to prepare by traditional methods. The azolium ions are potential cations for room temperature molten salts.

*Chemistry at the University of Bristol*, by LTC Chet Dymek, EOARD. (19 pp) [EOARD-LR-89-054]

The Chemistry Department at the University of Bristol is ranked among the top five in the U.K. It is very well equipped and the faculty members are both innovative and productive. Recently, three preproposals have come out of the department: (1) the synthesis of "molecular mats" or two-dimensional polymers; (2) new synthetic methods to form organosilicon compounds with substituents that are normally very reactive with organosilicons; and (3) the synthesis of anisotropic solids constructed from organo-metallic complexes. There were also strong groups studying the forces between adsorbed layers of polymers and the VUV spectroscopy and photochemistry of atoms and small molecules of interest in space and the ionosphere.

### Composite Materials

*Third European Conference on Composite Materials*, by LTC Chet Dymek and LTC James G.R. Hansen, EOARD. (19 pp) [EOARD-LR-89-050]

The Third European Conference on Composite Materials was held in Bordeaux, France, March 20-23, 1989. In terms of research reported, there was nearly equal representation from academia, and from industry and government laboratories. However, the attendance was heavily in favor of industry because of the approximately 120 exhibitors, including "giants" of the industry such as Rhone-Poulenc, SEP (near Bordeaux), and Aerospatiale. The subjects of the technical presentations were about equally divided among polymer, ceramic, and metal matrix composites. Areas receiving the greatest emphasis were SiC and carbon-containing composites, fiber structure and coatings, thermosets and thermoplastics, and laminate mechanics.

### Physics

*Laser Research at the Politecnico of Milan, Italy*, by Dr. Stacey Lazdinis, EOARD. (8 pp) [EOARD-LR-89-047]

The work is summarized of Professor Orazio Svelto and his colleagues at the Centro di Elettronica Quantistica e Strumentazione Elettronica in Milan, Italy, involving the development of highly efficient solid-state lasers, diffraction limited solid-state lasers, femto-second pulse generation, and biomedical laser applications.

### Telecommunications

*Aeritalia Space Systems Group*, by Dr. Vince Donlan, EOARD. (14 pp) [EOARD-LR-89-041]

Aeritalia has been involved in European space programs since the early 1960s. Space activities grew to the

point that in 1984 Aeritalia established a separate Space Systems Group (SSG) in Turin. Today, SSG is involved in dozens of projects, some of them jointly with NASA and U.S. aerospace companies. In this report, several of the major projects, such as the Tethered Satellite System, HIPPARCOS, Columbus Pressurized Module, Italian Research Interim Stage, and others are briefly described.

*Marconi Italiana*, by Dr. Vince Donlan, EOARD. (10 pp) [EOARD-LR-89-042]

Marconi Italiana specializes in military communications equipment such as digital switching equipment, digital multiplexers, cryptology equipment, and radios. In this report, technical specifications of two current Marconi products--a digital switch and a UHF multi-channel radio--are given; and some of Marconi's current R&D activities are described briefly.

*Selenia Spazio*, by Dr. Vince Donlan, EOARD. (6 pp) [EOARD-LR-89-043]

Selenia Spazio is a telecommunications technology company devoted exclusively to space programs--commercial, scientific, and military. The Rome plant is the main spacecraft integration facility; the L'Aquila plant produces the electronics--thick and thin film hybrid assemblies, printed circuit assemblies, gate array designs--and the antennas and reflectors; and the Catania plant specializes in the ground station equipment. This report describes some of the ongoing R&D efforts in the L'Aquila plant and lists some of the representative electronic, microelectronic, and microwave components that Selenia Spazio has designed and produced for various spacecraft.

## THE EMBASSIES: TECHNICAL ROUNDUP

### Federal Republic of Germany

*For further information on FRG items, contact Mr. Edward M. Malloy, Science Counselor, American Embassy, Bonn, APO New York 09080-7400.*

### Federal Republic of Germany Announces 5-Year Plan on Environmental Research

The Federal Republic of Germany (FRG) has approved a 5-year plan for environmental research and development. The plan, which should have little problem

obtaining legislative approval, emphasizes ecological research, the development of environmental technologies, and the sharing of expertise with developing countries.

On June 21, 1989, the federal cabinet adopted a program for "Environmental Research and Technology: 1989 to 1994," which provides a framework for environmental programs and policy for the next 5 years. Federal Minister for Research and Technology Heinz Riesenhuber announced a 1989 budget for the program of DM 550 million (\$290 million) to be increased by 4.2 percent annually.

The plan's guiding principle is the concept that early ecological research and technological realization are of decisive importance for successful, long-term environmental protection and that environmental policy should emphasize preventive rather than reactive measures. Research priorities will be the development of environmental protection technologies in the fields of emission reduction, purification of industrial exhausts, marine technologies, climate technology, and related subjects.

The new program emphasizes cooperation with developing countries. The FRG, on the basis of its own experience with environmental protection, is considered a suitable partner for developing countries facing environmental problems resulting from industrialization.

#### **Federal Republic of Germany's Science and Research Policy-1990 Draft Budget of the Federal Ministry for Research and Technology**

The FRG government's \$4 billion budget for the Ministry of Research and Technology (BMFT) calls for a healthy increase of five percent--substantially above the 3.4 percent increase asked for the overall federal budget. Virtually all the growth is accounted for in one sector--space. Included in this category are programs not only in nuclear and other energy sources, but also in information processing, electronics, microelectronics, production engineering, materials research, supersonic aviation, biotechnology, and ground transportation. General support for industrial research infrastructure is declining.

On July 7, the Federal Minister for Research and Technology, Dr. Heinz Riesenhuber, presented the draft budget for BMFT for 1990. Minister Riesenhuber pointed out that the highest growth rates go to the promotion of basic research, including large-scale research programs (research vessel meteor, the HERA accelerator, basic financing of the Max Planck Society), and the promotion of application-oriented basic research. Other areas with growing support are long-term research programs in the field of environment, polar and arctic research and space research as related to environmental monitoring, as well as health and gerontological research and other programs of future relevance.

Direct project support has been reduced under the BMFT budget in view of high research capabilities of German industries. Governmental support in favor of industrial promotion is now concentrated on support to medium-sized enterprises, on the strengthening of key technologies, including support of the research infrastructure of universities and research establishments, and on technology development in areas of public responsibility, such as reactor safety, transportation, and environment. Some examples are establishing centers for gene research, extending Fraunhofer Institutes for applied research in information and production technologies, establishing a Max Planck Institute for Polymer Research,

and establishing a German institute for artificial intelligence.

Under its energy research program, the FRG continues to spend less for nuclear energy and to increase its support for research on renewable energy sources. Energy generation and nuclear energy has set priorities on such areas as safety research, disposal of spent fuel elements, and new reactor concepts. In view of global climate changes and the necessary reduction of C0<sub>2</sub> emissions, the FRG government considers nuclear energy to remain an essential part of national and worldwide energy supply.

Under its space program, the federal government continues to support the development of European space programs as well as transatlantic cooperation, with initial steps also being taken regarding cooperation with the U.S.S.R. The 1990 funds are budgeted in line with the long-term ESA space plan (Ariane, Columbus, and HERMES), and the cooperation with NASA in the spacelab program. The funds budgeted for space research at a total of DM 1.466 billion cover 18.7 percent of the BMFT budget (13.6 percent in 1989) and thus lie below the range of funding for space research, which should not exceed 20 to 22 percent of the overall BMFT budget plan.

#### **France**

*For further information on French items, contact Dr. Allen Sessions, Science Counselor, American Embassy, Paris, APO New York 09777.*

#### **French Research and Its Relationship to the French Economy**

**Introduction.** This report asserts that French industry is not competitive enough in foreign markets and in its domestic market. Although French industry has improved since 1988, it has not resolved the two major problems confronting French economy--industrial employment and foreign trade deficit. The decline is caused by the deterioration of trade in manufactured goods. France has no market advantage compared to its competitors; it has no low prices as do Southeast Asian countries and no solid industrial structure like the Federal Republic of Germany (FRG). The only opportunity for France would be to exploit advanced technology. However, it appears that France has a lesser share in high-technology markets than its partners. A number of factors reflect France's weakness on high-technology markets: small number of patents taken by French researchers; income derived from licenses are among the lowest; sales and purchases of technology are low. French industry is weak, especially in medium- and high-technology areas. This is essentially because of insufficient industrial research. Further, cooperation between

public institutions and industrial corporations is hampered by low demand from French industrialists.

Until about 1980, France's scientific policy focused on scientific progress. The French government thought that such progress would automatically contribute to economic development. This policy helped France meet major technological challenges. The French government encouraged the creation of large corporations at the leading edge of technology and under governmental control. However, this proved to be incompatible with two other objectives: to ensure technology transfer between these corporations and from them to smaller firms, and the maintenance of the competitiveness of such corporations. Since 1980, the French government has realized the importance of industrial development across the corporate spectrum. To this end, various incentives now encourage innovative firms.

**A Strong Point of French Economy--The Large Programs.** The so-called large programs ("grands Programmes") concern sectors of major importance requiring long-term investments. There are four such large programs in the civilian sector--aeronautics, space, telecommunications, and nuclear. With the exception of aeronautics, each of these programs is the responsibility of ad hoc public research institutions: Centre National d'Etudes Sapieniales (CNES) [space], Centre National d'Etudes des Telecommunications (CNET) [telecommunications], and Commissariat d'Energie Atomique (CEA) [nuclear]. In aeronautics, there already existed old powerful industries. Therefore, the French government did not deem it necessary to create a public establishment in this sector. Observers have noted that, besides the U.S., only France and Japan enjoy exceptional technical advantages: Japan for all that concerns the penetration of leading-edge technologies into mass production, and France for major projects, whether national or European.

The four large programs do not cover all of France's major achievements. The difference between such programs and others such as the Train a Grande Vitesse (TGV) [high speed train] is that the latter were developed within existing structures. Such is also the case of military equipment.

Public research establishments are responsible for transferring to industry new technologies developed within the framework of the large programs. When there are no industrial partners, public establishments may create a new industry. Such is the case of CEA which created a powerful nuclear industry from scratch, and for CNES which constituted a space service industry (Arianespace and Spot Image).

**Strategic Industries Dependent on the Government: Electronics and Data Processing.** Electronics and data processing received 46 percent of the public funds allocated to industrial research. But Europe as a whole has

difficulty in resisting U.S. and Southeast Asian competition.

Electronics affects national independence and defense, which is why the fact that Europe is behind in these areas raises concerns (as it does in the U.S.). The situation is not made easier by the behavior of the major European corporations that hesitate between two policies: to constitute a competitive European industry or seek partnerships with U.S. or Japanese companies. In general, they choose the latter solution to simultaneously preserve their domestic market and access larger markets. It seems that France, Great Britain, and the FRG grant the same support to their industries--approximately F9 to 10 billion per year (\$1.3 to 1.5 billion). In data processing, Europe has been characterized by erratic national strategies.

**Industries Confronted with Competition.** Besides industries that receive important subsidies from the French government, there are others that are confronted with international competition with little public aid. In pharmacy, the research and development (R&D) expenditure/turnover ratio is 12.25 percent, ranking third after aeronautics and electronics. The volume of research still remains insufficient (five to seven times less than in the U.S. in 1982, half that of Japan, and less than the FRG and the U.K.). France went down from the second to the fifth rank for the discovery of new molecules and has a trade balance deficit in active substances.

Another example is that of automobile industry, but it is recovering. Its research budget, however, is less than that of some of France's competitors. Cooperative research is well-developed in that sector. Generally, the automobile industry benefits more than others from European Community (EC) programs and European Research Coordination Agency (EUREKA).

**Agriculture and Agrobusiness Industries.** Different from other industrial sectors, French agriculture was more able to benefit from new technologies. French agrobusiness industries, however, have not fully realized how important research is in agriculture. Compared with other industries, agrobusiness industries are tailenders with respect to research. About eight tenths of one percent of their added value is for research against 2.8 percent for the rest of French industry. Agrobusiness industries spend F6 billion (\$896 million) on advertisement and F1 billion (\$149 million) on research; that is less than Nestle alone and slightly more than General Foods. Industrialists are interested in augmenting their market shares through purchases or mergers rather than in creating more added value. In fact, French companies are slowly being absorbed by foreign corporations that conduct research outside of France.

With the exception of a few groups, agrobusiness industries are small and dispersed. They do little research

and are ill-prepared to take advantage of the explosion in new technologies.

France has a positive trade balance in agriculture. However, the added value of exported products is small. France exports large quantities of wheat but imports many products made from wheat. The expansion of agribusiness in France cannot overshadow its major weakness--insufficient research.

**Small- and Medium-Sized Companies.** The report distinguishes between those companies employing between 500 and a few thousands employees and those employing between 10 and 500 persons. The first category considers that research is a risk that must be taken by the government.

The 31,000 companies belonging to the second category represent 95 percent of the total of French industrial companies. The added value they bring represents two-thirds of that of large corporations. Thus, their role in the economy is important.

The French government has long ignored these companies and focused on large national corporations. In the 1970s, they realized that research conducted in public establishments and large corporations did not automatically lead to new products. Sometimes, smaller firms proved to be more innovative than larger companies.

The French government has only recently realized the importance of small firms. Small high-tech firms are innovative. Their managers often come from public laboratories or large corporations. They know how to find the information they need. Aside from these innovative firms, the great majority of small firms is ill-prepared to face the technological competition. They do not know how to find information.

France has no program to find ways to bring smaller firms out of their technological isolation. Firms are informed about new technologies through various channels. One of the most important is their contacts with larger corporations for which they act as subcontractors. The technological isolation of craftsmen is even greater than that of small firms.

**Collective Research and Industrial Technical Centers.** Collective research is research shared among several industrial companies. Between academic research (aimed at increasing knowledge) and industrial research (aimed at markets and development), basic technological and developmental research holds a key position. In general, small- and medium-sized firms do not have the financial and human resources or sometimes the desire to assume the risk of research. Collective research is the solution to this problem. Such research is essentially conducted by industrial technical centers. These centers have a total budget of F1,070 million (\$160 million) and employ 2,000 persons. Each center is closely connected with an industrial sector, with the greatest concentration of centers found in mechanics.

Center activities are distributed as follows: technological and development research-46 percent, technical aids, measures and test-10 percent, training and technology transfer-21 percent, standardization-6 percent, the remainder being constituted of miscellaneous tasks including circulation of information.

Various criticisms were addressed at these centers. One is that the distribution of centers between the Paris area and other regions of France favors more the latter, contrary to public research. Another criticism is that there is no communication between centers. Centers are also criticized as being bureaucratic. By 1992, France must reinforce its collective research.

**Governmental Action.** In order to improve technology transfer, directorates or units for the exploitation of research have been created in many public establishments. It is also possible for public establishments to create subsidiaries. The government has also taken various measures to support industrial research.

**Tax Incentives.** The French government can intervene through a tax incentive called "credit D'impôt Recherche" (research tax credit), allowing tax credits for companies equal to 25 percent of their increased R&D expenses. Created in 1983, this incentive turned out to be a success. Tax credits under this program amounted to F430 million (\$64 million) in 1984 and were granted to 1,600 companies. In 1987, 3,500 firms benefited from credits reaching F1,347 million (\$201 million). The research tax credit system encourages small- and medium-sized firms in general and involves a simple procedure that does not differentiate investments and operational expenditures and applies to both personnel and nonpersonnel expenses.

**National Programs.** The French government may also take measures reflecting governmental orientations. These are the so-called national programs, which are priority research programs over a period of 2 to 5 years. They must result in technological developments for industry or widen research fields.

Eleven programs with 33 projects were thus defined:

- To prepare the technologies of the future (biotechnologies, electronics and data processing, new materials and new chemistry)
- To increase the economic and social impact of research and technology (food, health, production technologies, national and regional development and transportation, natural resources)
- To know French society, particularly at the economic level, and to help developing countries.

**The Research and Technology Fund.** The Research Ministry uses the research and technology fund which permits the financing between two budgets of new technical and scientific programs that do not have come under any of the public research institutions. The 1989 fund's budget is F1,220 million (\$182 million) and is principally used for industrial research. In 1988, F600 million (\$89.5

million) went to the above-mentioned national programs. Funds are also available from the Industry Ministry and the Post and Telecommunications Ministry.

The multiplicity of financial aids has drawbacks. Potential beneficiaries do not always know what the best solution is. Further, there is confusion among French government officials and entities as to the global amount of the French government's effort.

**Agence Nationale pour la Valorisation de la Recherche [National Agency for the Exploitation of Research] (ANVAR).** The ANVAR principally focuses on the promotion of innovation, particularly with small- and medium-sized firms. The sectors receiving the strongest support are data processing-11.5 percent, the biomedical sector and agrobusiness-8.2 percent each, and consumer goods-6 percent.

The ANVAR currently employs 350 persons. Its 1989 budget is F150 million (\$22.4 million) for personnel and operational expenditures and F776 million (\$116 million) for projects.

**A Modernization Plan for Centre National de la Recherche Scientifique-National Center for Scientific Research.** Centre National de la Recherche Scientifique-National Center for Scientific Research (CNRS) is the largest and only multidisciplinary research establishment in France. The CNRS Director General, Francois Kourilsky, held a press conference on June 27, 1989, in which he presented the CNRS modernization plan. The CNRS activities are conducted through seven scientific directorates and by national institutes. The national committee of CNRS, which has an advisory role and is also responsible for evaluations, consists of 49 sections grouping various disciplines. One of the objectives of the modernization plan is to increase interaction between the various disciplines as well as discuss and disclose CNRS scientific strategies. To this end, various measures will be taken, such as the preparation of a 3-year plan that will be published in February 1990. Other measures include creating a directorate for strategy and programs. A review of the responsibilities of directorates with respect to content and interfaces with other directorates, increasing the number of interdisciplinary research projects (in such areas as new materials and environment), fostering multi-use technology research. The amount of financial support that will be given to the various disciplines and themes is currently being discussed.

The plan also aims at making CNRS more flexible and less bureaucratic in order to improve efficiency. The measures to meet this goal include reform of headquarters management as well as increased decentralization. However, evaluation and scientific policy remain the responsibility of CNRS headquarters.

Another objective of the modernization plan is to mobilize and motivate personnel. Various measures have already been taken, such as developing continued training (training budget was tripled) and creating a delegation for human resources. The problem of careers, promoting, and recruiting will also be reviewed.

The plan indicates that all CNRS laboratories must be given the means to conduct quality and competitive research. In the coming years, CNRS will concentrate on readjusting laboratory financial support. The creation or association of new laboratories will become dependent upon budgetary constraints. The criteria used to determine the excellence and appropriateness of future laboratories will become more strict. This budgetary strategy will imply that greater attention will be given to laboratories whose activities have declined.

The modernization plan emphasizes the need to increase interaction between CNRS and its partners--universities, grandes ecoles, companies, and regions. The CNRS also intends to further develop European cooperation. The creation of Club Des Organismes de Recherche et Assimiles-Club of Research and Research Related Organizations (CORA) at the Brussels CNRS office is a step in that direction. The CORA already groups several French research institutions. Consultations with other major European research institutions will be developed and relationships with European researchers and laboratories will be encouraged. The CNRS modernization procedures will be implemented by spring 1990.

For years, the CNRS reorganization has been a touchy subject. French officials and scientists agreed that CNRS was too cumbersome and too bureaucratic and was not able to quickly adjust to scientific developments. The various CNRS directors have tried to find solutions to this situation, but in vain. Kourilsky was very clear in this conference: the idea of getting rid of CNRS has been dropped. Whether Kourilsky will be successful in his endeavor remains to be seen. There are indeed areas where the reforms and adjustments advocated by the plan may be effective. However, CNRS will remain a public establishment with correlated budgetary constraints and personnel holding civil service status which precludes dismissal. One drawback is that salaries are in line with those paid to other civil servants which are relatively low. This status prevents mobility and dampens individual dynamism. Further, the fact that CNRS is a government organization necessarily limits the scope and nature of reforms in that these must take place within an established framework not subject to change. The Europe challenge, however, definitely constitutes an incentive to go beyond wishful thinking. In the end, it may well be the prospects of a united Europe that may force France to really do something about CNRS.

## Italy

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### Italian AIDS Update

According to the World Health Organization, Italy is now second to France in the number of AIDS cases in Europe, followed by the FRG, Spain, the U.K., Netherlands, Switzerland, Belgium, Denmark, and Sweden.

In Milan, the city in Italy with the highest number of AIDS cases, the rate of increase of the disease is slowing down. According to recent statistics in the first semester of 1989, only 4 Milanese per 100,000 developed AIDS versus 6 per 100,000 during the same period in 1988. In addition, it was found that in tests of drug addicts, the number of serum positive cases declined from 60 percent in 1986 to 38 percent in 1988.

The Italian Institute of Health is operating an AIDS Operating Center (Centro Operativo AIDS or COA) which is monitoring by computer the development of the disease in the 120 clinical centers where anti-AIDS therapies are conducted in over 2,500 cases.

A study conducted in 92 Italian hospitals of 39,102 newborn babies from September 1988 through March 1989 revealed that 1.33 babies per 1,000 were serum positive. About one third of these children develop AIDS. Of the 550,000 children born in Italy each year, about 720 should thus be serum positive, with about 240 likely to develop AIDS.

The Gruppo Italiano Cooperativo AIDS E Tumori (Italian Cooperative Group for AIDS and Tumors or GICAT), founded in 1986 to coordinate clinical research on the interaction between AIDS and tumors, has through September 1988 studied 435 cases of tumors associated to AIDS. Of these, 198 were Kaposi Sarcoma, 116 highly malignant non-Hodgkin Lymphoma, 20 other non-Hodgkin Lymphoma, 52 Hodgkin's disease, plus 49 cases of other types of Sarcoma and Leukemia.

A study conducted by the Italian Institute of Health in 11 hospitals indicates that a period of at least 12 months passes from the moment of infection to the first appearance of the AIDS virus. Serum positive cases develop AIDS at high rates between 12 and 30 months from the infection, while the rate of development remains constant between 30 and 60 months from the infection. Eighty percent of serum positive cases do not develop AIDS in the first 4 years from the date of infection.

Professor Giovanni Battista Rossi, Director of the Institute of Virology of the Institute of Health, said that the institute is beginning research on AIDS through experimentation on macaque monkeys.

The Italian National Research Council has approved a finalized research project on preventing and controlling

diseases with 97.7 billion lire (about \$70 million) for 5 years. One subproject is dedicated to research on new drugs for AIDS.

The government, in cooperation with the Administration of the Latium Region (Rome), approved a series of courses on AIDS for about 13,000 high school teachers. Taught by medical specialists, the teachers will pass their knowledge to the 525,000 students of the Latium region. The course was a great success with the teachers and will be extended to other regions.

Elio Parodi, an Italian deputy at the European Parliament, submitted a resolution calling for EEC cooperation on AIDS, including joint information campaigns, training of medical personnel, safeguards on the anonymity AIDS victims, a guarantee of equal work opportunity for those with AIDS, and cancelling of any planned AIDS tests at borders. The European Parliament adopted the resolution.

Italian legislation does not require a physician to inform the partner of a serum positive person of the danger of AIDS infection; it is considered a breach of professionalism. The issue was debated in a medical journal with the majority favoring supplying information about AIDS patients.

In June, the second national TV channel commenced a special nightly 1-hour program Monday through Thursday of information, interviews, and true stories of AIDS patients. The AIDS Operational Center of the Institute of Health has prepared two free, informational video cassettes--one directed to physicians and the other to hospital technicians and nurses.

Physicians working with AIDS patients have asked that their new work contract include a special monthly indemnity of 200,000 lire (about \$150) plus an additional 15 days of paid vacation. The Minister for Public Administration rejected the request.

The special free AIDS telephone hotline received over 59,000 telephone calls in 22 months. The hotline continues to receive around 100 telephone calls per day, with the average increasing significantly during press and radio/TV AIDS campaigns. Men are calling twice as much as women, while 70 percent of the telephone calls are from individuals 20 to 40 years old.

### STRIDE: Italian Technology Roundup, June/July 1989

**Verona to be Site of European Institute of Technology.** The European Institute of Technology (EIT), founded in February 1988 through the sponsorship of five industries (AT&T, ENICHEM, IBM Europe, Montedison, and Philips), has found a site in the city of Verona on premises donated by the city. The institute, created as a point of contact between European private industry and the university research community, will offer short courses, summer workshops and a program leading to a masters degree in technology management. For its first

activity, EIT is funding 35 research projects in biotechnology/pharmacology, information technology, and materials technology.

**INFN Gets Financing for Research Facilities.** The National Institute of Nuclear Physics received from the government for 1989-1993 1,800 billion lire (about \$1.3 billion). About 1,000 people will be employed to improve the 19 sections of INFN located in as many universities and to develop research in INFN's four national laboratories. Eighty billion lire are earmarked for the development of a new particle accelerator in Frascati. Named "ARES", this accelerator will attain one billion electron-volts and be employed to develop radio frequency and superconductivity technologies. The Gran Sasso Laboratory will get 200 billion lire for new equipment, while 20 billion each will go to the Padua Accelerator and to the new Cyclotron in Catania. The Geneva large electron-positron collider (LEP) project will receive 30 billion lire.

**Laboratory of Cosmic Physics Inaugurated in Naples.** The Italian Space Agency (ASI) inaugurated in Naples a cosmic physics laboratory with the support of several universities and astronomical and geophysical observatories. The laboratory will study new sophisticated techniques to analyze extraterrestrial matter for meteorites. The laboratory will also study cosmic sand suspended in space and the formation of molecules containing carbonium that might be the first step in the formation of living matter.

**Trieste Research Area Plans Intelligent Systems Institute.** The Trieste research area is planning to set up an advanced institute for the studies of the human brain. Professor Emilio Bizzi, the Italian neurophysiologist who directs the Department of Brain and Cognitive Sciences at MIT, will be the director. The institute plans research activities in the simulation of biological systems such as vision mechanisms, the control of movements, memory, cellular functions, and nervous system development, and will cooperate with artificial intelligence laboratories studying expert systems, robots, and artificial organs.

**Italian Southern Universities Form Consortium to Study Cosmic Radiation.** Nine universities of southern Italy have formed a consortium to create in the Basilicata region a research laboratory to study high energy cosmic radiation. Called South Italy Neutrino and Gamma Astronomy Observatory (SINGAO), the laboratory is scheduled for completion in 2 years and will work in close cooperation with the Grand Sasso Laboratory of the National Institute for Nuclear Physics (INFN).

**University Consortium Coordinates Superconductivity Research.** An Italian consortium is coordinating cooperation among the national research centers and laboratories in superconductivity research. The Inter-university Consortium for Physics of Matter (INFM), which comprises 33 Italian universities and about 2,000 researchers, is also cooperating with the recently ap-

proved Italian National Research Council's finalized project on superconductive and cryogenic technologies. The INFM recently received one billion lire (about \$740,000) from the Nuova-Samim Company for superconductivity research.

**New National Program for Bioelectronics.** The Italian Minister of Scientific and Technological Research announced the approval of a national research program for bioelectronics research. The program has 89.5 billion lire (about \$66 million) for the first 3 years plus 230 billion lire (about \$170 million) for 5 additional years. The program is divided into three areas: "neuronal and submicronic electronics" to study the possibility of emulating human brain functions; "proteic engineering" to develop biochips in which silicon will be replaced by organic proteic material; and "biosensors" to develop hybrids composed by organic and electronic material to be employed in medical diagnostics and environmental monitoring. About 26 percent of financing is reserved for training experts and researchers in this new field.

**Serono Institute Produces Human Growth Hormone.** The Serono Institute of Pharmacological Research announced it has produced through genetic engineering a human growth hormone whose absence causes dwarfism. The product is obtained by inserting the gene of the protein to be fabricated into the DNA of a mammal cell, which then synthesizes the protein. According to the institute, therapy for dwarfism can now rely on an unlimited quantity of pure product rather than depending on small quantities obtained from cellular extraction.

**Ultraviolet Laser Light Employed in Arteriosclerosis Therapy.** Researchers of the University of Florence and the Italian National Research Council's Institute of Quantum Physics, with the technical support of the electronic company "Elen," have built a device employing strong intensity ultraviolet laser light to destroy plaques obstructing arteries. The method for this "no pain therapy" was developed at a cost of 3 billion lire (about \$2.2 million) and is similar to devices developed in Los Angeles, Berlin, and Paris.

**Italian Pharmaceutical Company FIDIA Signs Research Corporation Agreement with Soviet Union.** The Italian pharmaceutical company FIDIA is building in Moscow under an agreement with the Soviet Agency of Sciences, an institute for research on new therapeutic drugs for nervous system pathologies. Known as the FIDIA All-Union Neurosciences Laboratories, the institute will develop research programs based on the work of Nobel Laureate Rita Levi-Montalcini in nerve growth factors (NGF). The FIDIA carries on similar research in its U.S.-based laboratory and is planning to sponsor researcher training and exchanges among the U.S., the Soviet Union, and Italy.

**Italy and China Build Laboratory on Everest.** The Italian Research Council is installing on Mount Everest

an aluminum pyramid to house experiments in astronomy, gravity, geodesy, and geology in cooperation with the Chinese Academy of Sciences. Several Italian universities will participate in the program. Located at 5,600 meters altitude, the pyramid has a 187-square meter base, is 8.4 meter tall and will house 20 researchers.

**Italy Building Renewable Energies Laboratory for Egypt.** Ansaldo's Center for Energy Studies signed a contract with Egypt's New and Renewable Energy Authority (NREA) for the construction in Cairo of a renewable energies laboratory for the study of solar, wind, photovoltaic, and biomass energy sources. The 2 billion-lire contract (about \$1.5 million), is part of a 21 billion-lire EEC project for Egypt. The contract will provide Italian technicians and knowledge to establish an alternative energies policy for new urban and industrial settlements in the desert.

**Italian Robot Exports Surpass Imports.** In 1988, Italian industry imported 345 robots from abroad out of a total 2,262 robots for the year. During the same period, Italy exported 650 robots with a net gain of 60 billion lire (about \$44 million). During that period, Italy moved from fifth to fourth place in the world for production (3,924 billion lire) and export (1,792 billion lire) gaining a 7.2 percent share of the world market. The Italian National Research Council hopes to make Italian robots still more competitive through its robotics research project with an investment of 60 billion lire (about \$50 million) over 5 years.

**Genoa's Research Consortium.** Genoa's research consortium supports small and medium industry of the Liguria region. It comprises more than 20 laboratories and research centers, with about 300 technicians and researchers. The consortium offers services in several industrial areas, including mechanics, electronics, chemicals, metallurgy, biology, and building sciences. The consortium has a well-equipped CAD center plus access to several data banks that link the consortium to the major research centers in Europe, the U.S., and Japan.

## United Kingdom

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### U.K. Secretary of State for Education and Science's First Major Science Policy Address

During summer 1989, U.K. Secretary of State for Education and Science, Kenneth Baker, delivered his first major policy address before a meeting of the Academia Europaea Plenary. The following points are a useful primer on British science and technology (S&T) policy.

- The historical trend has been towards an increasingly close involvement of the state with

science. The work and theories of scientists have become a major factor in determining economic progress and sustaining international security.

- While some European countries determine their overall scientific spending through a central science ministry, the U.K. has a dispersed system. Individual ministers determine their funding needs, negotiate their budgets with the Treasury, and spend according to the government's general strategy for civil research.
- To coordinate this system, new machinery has been set up. A high-level scientific advisory body, the Advisory Council on Science and Technology, advises the Prime Minister directly. Under the Prime Minister's chairmanship, collective ministerial consideration exists regarding national S&T priorities.
- The government's prime responsibility is for basic and strategic research. The government discharges its responsibility by funding research in universities and polytechnics (700 million pounds in 1989/90) and research councils (816 million pounds in 1989/90). That is the U.K. science base. (Note: Total spending on all civil research and development is some 2 billion pounds, including 1.1 billion pounds spent by the various departments.)
- S&T are core subjects in the U.K.'s new national school curriculum. For the first time, students must study these subjects up to age 16.
- The government wants to shift the balance of new research activity towards more commercially viable areas.
- The U.K.'s system of public funding of university research combines freedom of inquiry for the researcher with targeted funding to exploit the promising idea. Namely, from the general funds provided to universities, scientists pursue speculative and innovative research of their choice. When such research begins to bear fruit, the best is given additional support by the research councils. Although some argue that all or most university funds should be transferred to the research councils, the government believes that the plurality of funding sources inherent in the present system has merit.
- No one knows exactly how much of the general funds allocated to universities goes towards science base research; the universities funding council will remedy this situation beginning in 1990/91. Where the research councils support university research projects, the councils will be responsible for costs of their sponsored projects except academic salaries and premises costs.
- The government believes that some emphasis should be given to areas where a return to society seems more likely. When exploitability can be discerned in

basic or strategic research; e.g., fundamental research on low-dimensional solids, funding from the government's science base is appropriate.

- While the government does not intend to impose the sharp differentiation of a higher education institutions (the so-called R-T-X proposal) recommended by the advisory board for the research councils, it does believe that there should be a concentration of resources. To that end, the universities funding council is funding university research on an ever more selective basis. Every university department has been judged and given a rating for its research performance. Money is then distributed on the basis of those ratings. Not all universities will be able to sustain front rank research in all fields in the future; some may become predominantly teaching universities.
- The Advisory Board for the Research Councils (ABRC) will address the current system of peer review of scientific research in the U.K.
- In response to an ABRC recommendation that the government should fund several interdisciplinary research centers (IRCs), 17 have now been established or approved (all suggested and chosen by the scientific community) with current year funds at 28 million pounds.
- A recent study on the respective responsibilities of the research councils in biological sciences recommended that the existing five councils be totally amalgamated. This proposal would require legislation and the ABRC will present the recommendation to Secretary Baker.
- While the amount of money the government spends on civil research and development (R&D) (0.6 percent of GDP) is not out of line with other countries, U.K. industry funding on R&D (1 percent of GDP) does not compare well. Given the improved economic climate in the U.K. over the past 10 years, industry must now plough back more of its profits into R&D and not look to the taxpayers to foot the bill. The decision not to put governmental money into near-market research should cause this to occur.
- As part of its effort to achieve closer collaboration between industry and the science base, the government has: encouraged universities to seek additional private funds; placed intellectual property rights with institutions; and set up the link initiative to provide a framework for collaboration.
- International research collaboration is of growing importance, especially in relation to environmental issues. Hence, the government will spend 71 million pounds on environmental research; much will be devoted to international projects. Special programs include: work on ozone layer depletion; the biogeochemical ocean flux study in the oceans' absorption of carbon dioxide; the world ocean circulation experiment assessing the role of the ocean in modifying the earth's climate; global atmospheric modeling to understand climate change; and the analysis of data from the European remote sensing satellite measuring such things as ocean wave heights, surface temperatures, and surface winds.
- Aside from international environmental cooperation, more than 100 million pounds of the U.K.'s science base goes to a wide range of research within the European Community framework program.
- Many areas of research are bursting with opportunity and promise. Examples are: unravelling the mysteries of the human genome; advanced electron microscopy; advances in parallel computing; and how the growth and development of plants are affected by ambient temperatures.

### Recent U.K. Science and Technology Initiatives

**Introduction.** This article summarizes the U.K. Science and Engineering Research Council (SERC) initiatives from January through June 1989.

**LINK Programs.** The LINK initiative provides a mechanism by which the public sector in the form of research councils and government departments joins with private sector companies to peruse research programs. While most research will likely be in engineering, a significant number will be science areas. This was illustrated when the council considered a further ten proposals under this program and decided that the following eight should be submitted for approval to the LINK steering group: new catalysts and catalytic processes; design of high-speed mechanisms; ventilation, air conditioning and refrigeration; structural composites; biochemical engineering; plant metabolism control; protein engineering; and nanotechnology.

**Government and Industry Fund Virus Research Unit.** A new research unit called the Virus Molecular Biology Group and directed by Drs. Susan and Alan Kingsman has been established in Oxford's Biochemistry Department as a result of a major investment by Glaxo Group Research and British Biotechnology Ltd., together with SERC's Biotechnology Directorate and the Department of Trade and Industry. The research goal is to determine how viruses invade human cells and dominate them to cause serious disease.

During the next 4 years, the Oxford team will isolate individual genes from two types of viruses--papilloma-viruses associated with human cervical cancer and retro-viruses associated with diseases such as AIDS and leukemia.

Scientists in the group have already developed new ways of studying the protein products of these viruses. They can "force" simple microbes to make large quantities of each type of protein from human viruses. They can also "force" the proteins to function correctly in simple cells by using sophisticated genetic engineering techniques. The first promising results of this technology have already been achieved. The group has purified one of the proteins that plays a key role in the AIDS virus life cycle. This protein has many functions and, by measuring its effects in different cell types, the group is beginning to identify the essential properties of this important protein. In the long term, it is hoped that this new knowledge may lead to the development of more effective methods for analyzing compounds that block HIV replication in human cells.

**LINK Program for Collaborative Research in Design of High-Speed Machinery.** A program to promote pre-competitive collaborative research leading to advances in the design of high-speed and high-performance machinery has been approved. The program, supported by SERC and the Department of Trade and Industry, will cost 20 million pounds. It will focus on the development of a modular design approach, based on the unifying concept of distributed microprocessor controlled drives. It will exploit the base of expertise in academia and industry through a coordinated program of precompetitive research projects directed towards machine element packages required for the future generation of flexible and adaptable machines. Increases in speed, quality, and variety will be the central objectives, concentrating on research applicable to the following sectors: assembly and handling machinery; computer equipment; leatherworking and footwear machinery; metal-cutting machine tools; metal-form machinery; mining, earthmoving, and construction machinery; packaging machinery; paper- and board-making machinery; printing machinery; and textile machinery. This program offers the prospect of significant improvements in the design and performance of a wide range of process machinery.

**U.K. and FRG Collaborate on a New Instrument for ISIS.** Federal Republic of Germany and British scientists have agreed to collaborate on a new type of spectrometer to be installed at the ISIS Neutron Facility at SERC's Rutherford Appleton Laboratory (RAL) in Oxfordshire. The new one million-pound instrument called ROTAX will be used to determine the properties of materials. The ROTAX is a new type of crystal analyzer time-of-flight spectrometer for elastic and inelastic scattering measurements at a pulsed neutron source. The ROTAX incorporates a novel, nonuniformly rotating analyzer system, and will be used to measure collective excitations such as phonons and magnons in single crystals. This research has usually been carried out at reactors using the so-called triple axis spectrometer. When it begins operating in 1991, ROTAX will be a valuable addition to the exist-

ing range of 13 instruments available at ISIS. These cover an unparalleled energy and resolution range for neutron-scattering research, and ensure the position of ISIS as one of the world's most advanced pulsed neutron source.

There are already several German collaborations at ISIS, including the Karmen Neutrino Experiment and the Joint European Pulsed Muon Facility. The spectrometer design was developed by a group at the University of Wurzburg led by Professor Reinhart Geick. Work on the prototype began early last year at Wurzburg. Scientists from RAL and U.K. universities will be involved in its installation and exploitation at ISIS. The ISIS is probably the world's leading high intensity pulsed neutron facility, primarily used for condensed matter research using slow neutron scattering techniques. It also serves the Neutrino Facility Karmen, a collaborative venture with KFK Karlsruhe, and the European pulsed Muon Facility, a collaboration among France, Germany, Italy, Sweden, and the U.K., supported in part by the EC.

**U.K. Contribution to LEP.** In summer 1989, one of the major world scientific instruments, the large electron positron collider (LEP) at the European Laboratory for Particle Physics (CERN) in Geneva, was completed costing one billion Swiss francs. The LEP is housed in a 27-KM circumference tunnel under the French and Swiss countryside. The LEP is designed specifically to study the Z and W particles, which are associated with the weak force, one of nature's four fundamental forces.

The U.K. was one of the founding members of CERN and the current U.K. subscription (45 million pounds) is paid on behalf of the U.K. government by SERC. The SERC has also been supporting the U.K. academic groups that are heavily involved in three out of the four experiments--ALEPH, DELPHI and OPAL--through research grants and through RAL which has supplied engineering, design, computational, and theoretical physics expertise. The SERC contributions have been about 30 million pounds over the last 8 years.

**New U.K. Biotechnology Programs.** The U.K. has launched a new 5-year, 7.5 million-pound research program that will increase industrial use of biotechnology. The biochemical engineering program, part of the government's LINK initiative, will support collaboration between industry and the scientific community. Government funding will be provided by the DTI (4.3 million pounds) and SERC (3.2 million pounds). Individual projects will be funded 50/50 by industry and government. Biochemical engineering is concerned with the development of equipment and processes to exploit biotechnology on an industrial scale. The program will address four priority areas:

- Innovative downstream processing: research into novel processes and equipment for enhanced product recovery

- Fermentation technology: development of new and improved fermenter designs
- Process control in biotechnology: creation of control technology for the auto regulation, organization, and integration of bioprocesses
- Containment, asepsis, sterility, and the environment: improved barrier technologies for exclusion of external environment from sensitive bioprocesses and containment of potentially hazardous agents within bioprocesses.

**LINK Program on Catalysts and Catalytic Processes.** The U.K. government has announced a new 5 million-pound program, under the LINK initiative, for collaborative research into new catalysts and catalytic processes. Government funding of 2.5 million pounds will be shared equally between DTI and SERC over a 5-year period. This funding will be matched by contributions from industry towards individual projects.

The program will focus on seven areas of research:

- C1 chemistry conversions: including conversion of syngas or methane to higher value products
- Hydrocarbon processing: e.g., catalytic cracking of fuel oils in the refining process
- Environmental control: improved industrial effluent control and vehicle exhaust systems
- Electrocatalytic technology: e.g., fuel CEL for clean power generation
- Photocatalysis: including improved water purification techniques
- Polymerization: novel polymerization catalysis
- Enabling technologies for catalysis: e.g., research into methods of catalyst regeneration.

Forty-six industrial and seventeen science-based organizations are interested in catalysis research. Organizations likely to participate in early projects include Liverpool Polytechnic, UMIST, British Gas, ICI, and Johnson Matthey.

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24	4539	Solid-State Physics . . . . .	Dr. Dean L. Mitchell
51	402-2471	Information Science . . . . .	Dr. Jack F. Blackburn